|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Name | SMILES | InChI | Structure | Formula |
| H | [H] | InChI=1S/H |

|  |
| --- |
|  |

 | H |
| H2 | [H][H] | InChI=1S/H2/h1H |  | H2 |
| O | [O] | InChI=1S/O | C:\Users\Administrator\AppData\Local\Temp\mx38D3C.png | O |
| O2 | [O][O] | InChI=1S/O2/c1-2 |  | O2 |
| OH | [OH] | InChI=1S/HO/h1H |  | HO |
| OH\* | [OH] | InChI=1S/HO/h1H |  | HO |
| H2O | O | InChI=1S/H2O/h1H2 |  | H2O |
| N2 | N#N | InChI=1S/N2/c1-2 |  | N2 |
| HO2 | [O]O | InChI=1S/HO2/c1-2/h1H |  | HO2 |
| H2O2 | OO | InChI=1S/H2O2/c1-2/h1-2H |  | H2O2 |
| AR | [Ar] | InChI=1S/Ar |  | AR |
| CO | [C]=O | InChI=1S/CO/c1-2 | C:\Users\Administrator\AppData\Local\Temp\mx3157E.png | CO |
| CO2 | O=C=O | InChI=1S/CO2/c2-1-3 |  | CO2 |
| CH2O | C=O | InChI=1S/CH2O/c1-2/h1H2 |  | CH2O |
| HCO | [CH]=O | InChI=1S/CHO/c1-2/h1H |  | CHO |
| HO2CHO | O=COO | InChI=1S/CH2O3/c2-1-4-3/h1,3H |  | CH2O3 |
| HCOH | singlet[CH]O | InChI=1S/CH2O/c1-2/h1-2H | C:\Users\Administrator\AppData\Local\Temp\mx3B084.png | CH2O |
| O2CHO | [O]OC=O | InChI=1S/CHO3/c2-1-4-3/h1H |  | CHO3 |
| HOCHO | O=CO | InChI=1S/CH2O2/c2-1-3/h1H,(H,2,3) |  | CH2O2 |
| OCHO | [O]C=O | InChI=1S/CHO2/c2-1-3/h1H |  | CHO2 |
| HOCH2O2H | OCOO | InChI=1S/CH4O3/c2-1-4-3/h2-3H,1H2 |  | CH4O3 |
| HOCH2O2 | [O]OCO | InChI=1S/CH3O3/c2-1-4-3/h2H,1H2 |  | CH3O3 |
| OCH2O2H | [O]COO | InChI=1S/CH3O3/c2-1-4-3/h3H,1H2 |  | CH3O3 |
| HOCH2O | [O]CO | InChI=1S/CH3O2/c2-1-3/h2H,1H2 |  | CH3O2 |
| CH3OH | CO | InChI=1S/CH4O/c1-2/h2H,1H3 |  | CH4O |
| CH2OH | [CH2]O | InChI=1S/CH3O/c1-2/h2H,1H2 |  | CH3O |
| CH3O | C[O] | InChI=1S/CH3O/c1-2/h1H3 |  | CH3O |
| CH3O2H | COO | InChI=1S/CH4O2/c1-3-2/h2H,1H3 |  | CH4O2 |
| CH3O2 | CO[O] | InChI=1S/CH3O2/c1-3-2/h1H3 |  | CH3O2 |
| CH4 | C | InChI=1S/CH4/h1H4 |  | CH4 |
| CH3 | [CH3] | InChI=1S/CH3/h1H3 |  | CH3 |
| CH2 | triplet[CH2] | InChI=1S/CH2/h1H2 | C:\Users\Administrator\AppData\Local\Temp\mx31FBA.png | CH2 |
| CH2(S) | singlet[CH2] | InChI=1S/CH2/h1H2 | C:\Users\Administrator\AppData\Local\Temp\mx31FBA.png | CH2 |
| C | [C] | InChI=1S/C | C:\Users\Administrator\AppData\Local\Temp\mx3D581.png | C |
| CH | [CH] | InChI=1S/CH/H1h |  | CH |
| CH\* | [CH] | InChI=1S/CH/H1h |  | CH |
| C2H6 | CC | InChI=1S/C2H6/c1-2/h1-2H3 |  | C2H6 |
| C2H5 | [CH2]C | InChI=1S/C2H5/c1-2/h1H2,2H3 |  | C2H5 |
| C2H4 | C=C | InChI=1S/C2H4/c1-2/h1-2H2 |  | C2H4 |
| C2H3 | [CH]=C | InChI=1S/C2H3/c1-2/h1H,2H2 |  | C2H3 |
| C2H2 | C#C | InChI=1S/C2H2/c1-2/h1-2H |  | C2H2 |
| C2H | [C]#C | InChI=1S/C2H/c1-2/h1H |  | C2H |
| CH3CHO | CC=O | InChI=1S/C2H4O/c1-2-3/h2H,1H3 |  | C2H4O |
| C2H3OH | C=CO | InChI=1S/C2H4O/c1-2-3/h2-3H,1H2 |  | C2H4O |
| C2H2OH | [CH]=CO | InChI=1S/C2H3O/c1-2-3/h1-3H |  | C2H3O |
| CH3CO | C[C]=O | InChI=1S/C2H3O/c1-2-3/h1H3 |  | C2H3O |
| CH2CHO | [CH2]C=O | InChI=1S/C2H3O/c1-2-3/h2H,1H2 |  | C2H3O |
| O2CH2CHO | [O]OCC=O | InChI=1S/C2H3O3/c3-1-2-5-4/h1H,2H2 |  | C2H3O3 |
| HO2CH2CO | O=[C]COO | InChI=1S/C2H3O3/c3-1-2-5-4/h4H,2H2 |  | C2H3O3 |
| CH2CO | C=C=O | InChI=1S/C2H2O/c1-2-3/h1H2 |  | C2H2O |
| HCCO | [CH]=C=O | InChI=1S/C2HO/c1-2-3/h1H |  | C2HO |
| HCCOH | C#CO | InChI=1S/C2H2O/c1-2-3/h1,3H |  | C2H2O |
| CH3CO3H | CC(=O)OO | InChI=1S/C2H4O3/c1-2(3)5-4/h4H,1H3 |  | C2H4O3 |
| CH3CO3 | CC(=O)O[O] | InChI=1S/C2H3O3/c1-2(3)5-4/h1H3 |  | C2H3O3 |
| CH3CO2 | CC([O])=O | InChI=1S/C2H3O2/c1-2(3)4/h1H3 |  | C2H3O2 |
| C2H5OH | CCO | InChI=1S/C2H6O/c1-2-3/h3H,2H2,1H3 |  | C2H6O |
| C2H5O | CC[O] | InChI=1S/C2H5O/c1-2-3/h2H2,1H3 |  | C2H5O |
| PC2H4OH | [CH2]CO | InChI=1S/C2H5O/c1-2-3/h3H,1-2H2 |  | C2H5O |
| SC2H4OH | C[CH]O | InChI=1S/C2H5O/c1-2-3/h2-3H,1H3 |  | C2H5O |
| O2C2H4OH | [O]OCCO | InChI=1S/C2H5O3/c3-1-2-5-4/h3H,1-2H2 |  | C2H5O3 |
| C2H5O2H | CCOO | InChI=1S/C2H6O2/c1-2-4-3/h3H,2H2,1H3 |  | C2H6O2 |
| C2H5O2 | CCO[O] | InChI=1S/C2H5O2/c1-2-4-3/h2H2,1H3 |  | C2H5O2 |
| C2H4O2H | [CH2]COO | InChI=1S/C2H5O2/c1-2-4-3/h3H,1-2H2 |  | C2H5O2 |
| C2H4O1-2 | C1CO1 | InChI=1S/C2H4O/c1-2-3-1/h1-2H2 |  | C2H4O |
| C2H3O1-2 | [CH]1CO1 | InChI=1S/C2H3O/c1-2-3-1/h1H,2H2 |  | C2H3O |
| CH3COCH3 | CC(C)=O | InChI=1S/C3H6O/c1-3(2)4/h1-2H3 |  | C3H6O |
| CH3COCH2 | [CH2]C(C)=O | InChI=1S/C3H5O/c1-3(2)4/h1H2,2H3 |  | C3H5O |
| CH3COCH2O2 | CC(=O)CO[O] | InChI=1S/C3H5O3/c1-3(4)2-6-5/h2H2,1H3 |  | C3H5O3 |
| C3KET21 | CC(=O)COO | InChI=1S/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3 |  | C3H6O3 |
| C2H3CHO | C=CC=O | InChI=1S/C3H4O/c1-2-3-4/h2-3H,1H2 |  | C3H4O |
| C2H3CO | C=C[C]=O | InChI=1S/C3H3O/c1-2-3-4/h2H,1H2 |  | C3H3O |
| C2H5CHO | CCC=O | InChI=1S/C3H6O/c1-2-3-4/h3H,2H2,1H3 |  | C3H6O |
| C2H5CO | CC[C]=O | InChI=1S/C3H5O/c1-2-3-4/h2H2,1H3 |  | C3H5O |
| CH3OCH3 | COC | InChI=1S/C2H6O/c1-3-2/h1-2H3 |  | C2H6O |
| CH3OCH2 | [CH2]OC | InChI=1S/C2H5O/c1-3-2/h1H2,2H3 |  | C2H5O |
| CH3OCH2O2 | COCO[O] | InChI=1S/C2H5O3/c1-4-2-5-3/h2H2,1H3 |  | C2H5O3 |
| CH2OCH2O2H | [CH2]OCOO | InChI=1S/C2H5O3/c1-4-2-5-3/h3H,1-2H2 |  | C2H5O3 |
| CH3OCH2O2H | COCOO | InChI=1S/C2H6O3/c1-4-2-5-3/h3H,2H2,1H3 |  | C2H6O3 |
| CH3OCH2O | COC[O] | InChI=1S/C2H5O2/c1-4-2-3/h2H2,1H3 |  | C2H5O2 |
| O2CH2OCH2O2H | [O]OCOCOO | InChI=1S/C2H5O5/c3-6-1-5-2-7-4/h3H,1-2H2 |  | C2H5O5 |
| HO2CH2OCHO | O=COCOO | InChI=1S/C2H4O4/c3-1-5-2-6-4/h1,4H,2H2 |  | C2H4O4 |
| OCH2OCHO | [O]COC=O | InChI=1S/C2H3O3/c3-1-5-2-4/h1H,2H2 |  | C2H3O3 |
| HOCH2OCO | O=[C]OCO | InChI=1S/C2H3O3/c3-1-5-2-4/h3H,1H2 |  | C2H3O3 |
| CH3OCHO | COC=O | InChI=1S/C2H4O2/c1-4-2-3/h2H,1H3 |  | C2H4O2 |
| CH3OCO | CO[C]=O | InChI=1S/C2H3O2/c1-4-2-3/h1H3 |  | C2H3O2 |
| CH2OCHO | [CH2]OC=O | InChI=1S/C2H3O2/c1-4-2-3/h2H,1H2 |  | C2H3O2 |
| HE | [He] | InChI=1S/He |  | HE |
| C3H8 | CCC | InChI=1S/C3H8/c1-3-2/h3H2,1-2H3 |  | C3H8 |
| IC3H7 | C[CH]C | InChI=1S/C3H7/c1-3-2/h3H,1-2H3 |  | C3H7 |
| NC3H7 | [CH2]CC | InChI=1S/C3H7/c1-3-2/h1,3H2,2H3 |  | C3H7 |
| C3H6 | C=CC | InChI=1S/C3H6/c1-3-2/h3H,1H2,2H3 |  | C3H6 |
| C3H5-A | [CH2]C=C | InChI=1S/C3H5/c1-3-2/h3H,1-2H2 |  | C3H5 |
| C3H5-S | [CH]=CC | InChI=1S/C3H5/c1-3-2/h1,3H,2H3 |  | C3H5 |
| C3H5-T | C=[C]C | InChI=1S/C3H5/c1-3-2/h1H2,2H3 |  | C3H5 |
| C3H4-P | C#CC | InChI=1S/C3H4/c1-3-2/h1H,2H3 |  | C3H4 |
| C3H4-A | C=C=C | InChI=1S/C3H4/c1-3-2/h1-2H2 |  | C3H4 |
| C3H3 | C#C[CH2] | InChI=1S/C3H3/c1-3-2/h1H,2H2 |  | C3H3 |
| C3H5O | C=CC[O] | InChI=1S/C3H5O/c1-2-3-4/h2H,1,3H2 |  | C3H5O |
| C3H6OOH1-2 | C[CH]COO | InChI=1S/C3H7O2/c1-2-3-5-4/h2,4H,3H2,1H3 |  | C3H7O2 |
| C3H6OOH1-3 | [CH2]CCOO | InChI=1S/C3H7O2/c1-2-3-5-4/h4H,1-3H2 |  | C3H7O2 |
| C3H6OOH2-1 | [CH2]C(C)OO | InChI=1S/C3H7O2/c1-3(2)5-4/h3-4H,1H2,2H3 |  | C3H7O2 |
| C3H6OOH1-2O2 | CC(COO)O[O] | InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-4H,2H2,1H3 |  | C3H7O4 |
| C3H6OOH1-3O2 | [O]OCCCOO | InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h4H,1-3H2 |  | C3H7O4 |
| C3H6OOH2-1O2 | CC(CO[O])OO | InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3,5H,2H2,1H3 |  | C3H7O4 |
| NC3H7O2H | CCCOO | InChI=1S/C3H8O2/c1-2-3-5-4/h4H,2-3H2,1H3 |  | C3H8O2 |
| IC3H7O2H | CC(C)OO | InChI=1S/C3H8O2/c1-3(2)5-4/h3-4H,1-2H3 |  | C3H8O2 |
| NC3H7O2 | CCCO[O] | InChI=1S/C3H7O2/c1-2-3-5-4/h2-3H2,1H3 |  | C3H7O2 |
| IC3H7O2 | CC(C)O[O] | InChI=1S/C3H7O2/c1-3(2)5-4/h3H,1-2H3 |  | C3H7O2 |
| NC3H7O | CCC[O] | InChI=1S/C3H7O/c1-2-3-4/h2-3H2,1H3 |  | C3H7O |
| IC3H7O | CC(C)[O] | InChI=1S/C3H7O/c1-3(2)4/h3H,1-2H3 |  | C3H7O |
| C3H6O1-2 | CC1CO1 | InChI=1S/C3H6O/c1-3-2-4-3/h3H,2H2,1H3 |  | C3H6O |
| C3H6O1-3 | C1COC1 | InChI=1S/C3H6O/c1-2-4-3-1/h1-3H2 |  | C3H6O |
| C3KET12 | CC(C=O)OO | InChI=1S/C3H6O3/c1-3(2-4)6-5/h2-3,5H,1H3 |  | C3H6O3 |
| C3KET13 | O=CCCOO | InChI=1S/C3H6O3/c4-2-1-3-6-5/h2,5H,1,3H2 |  | C3H6O3 |
| C3H51-2,3OOH | [CH2]C(COO)OO | InChI=1S/C3H7O4/c1-3(7-5)2-6-4/h3-5H,1-2H2 |  | C3H7O4 |
| C3H52-1,3OOH | OOC[CH]COO | InChI=1S/C3H7O4/c4-6-2-1-3-7-5/h1,4-5H,2-3H2 |  | C3H7O4 |
| C3H5O1-2OOH-3 | C1C(O1)C(OO) | InChI=1S/C3H6O3/c4-6-2-3-1-5-3/h3-4H,1-2H2 |  | C3H6O3 |
| C3H5O1-3OOH-2 | C1C(OO)C(O1) | InChI=1S/C3H6O3/c4-6-3-1-5-2-3/h3-4H,1-2H2 |  | C3H6O3 |
| C3H6OH1-2 | C(O)[CH]C | InChI=1S/C3H7O/c1-2-3-4/h2,4H,3H2,1H3 |  | C3H7O |
| CH3CHCO | CC=C=O | InChI=1S/C3H4O/c1-2-3-4/h2H,1H3 |  | C3H4O |
| AC3H5OOH | C=CCOO | InChI=1S/C3H6O2/c1-2-3-5-4/h2,4H,1,3H2 |  | C3H6O2 |
| C2H3OOH | C=COO | InChI=1S/C2H4O2/c1-2-4-3/h2-3H,1H2 |  | C2H4O2 |
| CC3H4 | C1=CC1 | InChI=1S/C3H4/c1-2-3-1/h1-2H,3H2 |  | C3H4 |
| H2CC | [C]=C | InChI=1S/C2H2/c1-2/H1h2 |  | C2H2 |
| FULVENE | C=C1C=CC=C1 | InChI=1S/C6H6/c1-6-4-2-3-5-6/h2-5H,1H2 |  | C6H6 |
| CC3H6 | C1CC1 | InChI=1S/C3H6/c1-2-3-1/h1-3H2 |  | C3H6 |
| C4H10 | CCCC | InChI=1S/C4H10/c1-3-4-2/h3-4H2,1-2H3 |  | C4H10 |
| C4H8-1 | C=CCC | InChI=1S/C4H8/c1-3-4-2/h3H,1,4H2,2H3 |  | C4H8 |
| C4H8-2 | CC=CC | InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3 |  | C4H8 |
| PC4H9 | [CH2]CCC | InChI=1S/C4H9/c1-3-4-2/h1,3-4H2,2H3 |  | C4H9 |
| SC4H9 | C[CH]CC | InChI=1S/C4H9/c1-3-4-2/h3H,4H2,1-2H3 |  | C4H9 |
| C4H71-1 | [CH]=CCC | InChI=1S/C4H7/c1-3-4-2/h1,3H,4H2,2H3 |  | C4H7 |
| C4H71-2 | C=[C]CC | InChI=1S/C4H7/c1-3-4-2/h1,4H2,2H3 |  | C4H7 |
| C4H71-3 | C=C[CH]C | InChI=1S/C4H7/c1-3-4-2/h3-4H,1H2,2H3 |  | C4H7 |
| C4H71-4 | [CH2]CC=C | InChI=1S/C4H7/c1-3-4-2/h3H,1-2,4H2 |  | C4H7 |
| C4H72-2 | C[C]=CC | InChI=1S/C4H7/c1-3-4-2/h3H,1-2H3 |  | C4H7 |
| C4H6 | C=CC=C | InChI=1S/C4H6/c1-3-4-2/h3-4H,1-2H2 |  | C4H6 |
| PC4H9O2H | CCCCOO | InChI=1S/C4H10O2/c1-2-3-4-6-5/h5H,2-4H2,1H3 |  | C4H10O2 |
| SC4H9O2H | CCC(C)OO | InChI=1S/C4H10O2/c1-3-4(2)6-5/h4-5H,3H2,1-2H3 |  | C4H10O2 |
| PC4H9O2 | CCCCO[O] | InChI=1S/C4H9O2/c1-2-3-4-6-5/h2-4H2,1H3 |  | C4H9O2 |
| SC4H9O2 | CCC(C)O[O] | InChI=1S/C4H9O2/c1-3-4(2)6-5/h4H,3H2,1-2H3 |  | C4H9O2 |
| PC4H9O | CCCC[O] | InChI=1S/C4H9O/c1-2-3-4-5/h2-4H2,1H3 |  | C4H9O |
| SC4H9O | CCC(C)[O] | InChI=1S/C4H9O/c1-3-4(2)5/h4H,3H2,1-2H3 |  | C4H9O |
| C4H71-O | C=CC([O])C | InChI=1S/C4H7O/c1-3-4(2)5/h3-4H,1H2,2H3 |  | C4H7O |
| C4H8O1-2 | CCC1CO1 | InChI=1S/C4H8O/c1-2-4-3-5-4/h4H,2-3H2,1H3 |  | C4H8O |
| C4H8O1-3 | CC1CCO1 | InChI=1S/C4H8O/c1-4-2-3-5-4/h4H,2-3H2,1H3 |  | C4H8O |
| C4H8O1-4 | C1CCOC1 | InChI=1S/C4H8O/c1-2-4-5-3-1/h1-4H2 |  | C4H8O |
| C4H8O2-3 | CC1OC1C | InChI=1S/C4H8O/c1-3-4(2)5-3/h3-4H,1-2H3 |  | C4H8O |
| SC4H8OH-3 | CC(O)[CH]C | InChI=1S/C4H9O/c1-3-4(2)5/h3-5H,1-2H3 |  | C4H9O |
| C4H8OH-1O2 | CCC(CO)O[O] | InChI=1S/C4H9O3/c1-2-4(3-5)7-6/h4-5H,2-3H2,1H3 |  | C4H9O3 |
| C4H8OH-2O2 | CCC(C)(O)O[O] | InChI=1S/C4H9O3/c1-3-4(2,5)7-6/h5H,3H2,1-2H3 |  | C4H9O3 |
| C4H8OOH1-2 | CC[CH]COO | InChI=1S/C4H9O2/c1-2-3-4-6-5/h3,5H,2,4H2,1H3 |  | C4H9O2 |
| C4H8OOH1-3 | C[CH]CCOO | InChI=1S/C4H9O2/c1-2-3-4-6-5/h2,5H,3-4H2,1H3 |  | C4H9O2 |
| C4H8OOH1-4 | [CH2]CCCOO | InChI=1S/C4H9O2/c1-2-3-4-6-5/h5H,1-4H2 |  | C4H9O2 |
| C4H8OOH2-1 | [CH2]C(CC)OO | InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,2-3H2,1H3 |  | C4H9O2 |
| C4H8OOH2-3 | C[CH]C(C)OO | InChI=1S/C4H9O2/c1-3-4(2)6-5/h3-5H,1-2H3 |  | C4H9O2 |
| C4H8OOH2-4 | [CH2]CC(C)OO | InChI=1S/C4H9O2/c1-3-4(2)6-5/h4-5H,1,3H2,2H3 |  | C4H9O2 |
| C4H8OOH1-2O2 | CCC(COO)O[O] | InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4-5H,2-3H2,1H3 |  | C4H9O4 |
| C4H8OOH1-3O2 | CC(CCOO)O[O] | InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4-5H,2-3H2,1H3 |  | C4H9O4 |
| C4H8OOH1-4O2 | [O]OCCCCOO | InChI=1S/C4H9O4/c5-7-3-1-2-4-8-6/h5H,1-4H2 |  | C4H9O4 |
| C4H8OOH2-1O2 | CCC(CO[O])OO | InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4,6H,2-3H2,1H3 |  | C4H9O4 |
| C4H8OOH2-3O2 | CC(O[O])C(C)OO | InChI=1S/C4H9O4/c1-3(7-5)4(2)8-6/h3-5H,1-2H3 |  | C4H9O4 |
| C4H8OOH2-4O2 | CC(CCO[O])OO | InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4,6H,2-3H2,1H3 |  | C4H9O4 |
| C4H72-1OOH | CC=CCOO  | InChI=1S/C4H8O2/c1-2-3-4-6-5/h2-3,5H,4H2,1H3 |  | C4H8O2 |
| C4H71-4OOH | C=CCCOO  | InChI=1S/C4H8O2/c1-2-3-4-6-5/h2,5H,1,3-4H2 |  | C4H8O2 |
| C4H71-3OOH | C=CC(C)OO  | InChI=1S/C4H8O2/c1-3-4(2)6-5/h3-5H,1H2,2H3 |  | C4H8O2 |
| C4H71-3,4OOH | [CH2]CC(OO)C(OO) | InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h4-6H,1-3H2 |  | C4H9O4 |
| C4H72-3,4OOH | C[CH]C(OO)C(OO) | InChI=1S/C4H9O4/c1-2-4(8-6)3-7-5/h2,4-6H,3H2,1H3 |  | C4H9O4 |
| C4H71-2,4OOH | [CH2]C(OO)CC(OO) | InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h4-6H,1-3H2 |  | C4H9O4 |
| C4H72-1,3OOH | CC(OO)[CH]C(OO) | InChI=1S/C4H9O4/c1-4(8-6)2-3-7-5/h2,4-6H,3H2,1H3 |  | C4H9O4 |
| C4H72-1,4OOH | C(OO)C[CH]C(OO) | InChI=1S/C4H9O4/c5-7-3-1-2-4-8-6/h1,5-6H,2-4H2 |  | C4H9O4 |
| C4H71-2,3OOH | [CH2]C(OO)C(OO)C | InChI=1S/C4H9O4/c1-3(7-5)4(2)8-6/h3-6H,1H2,2H3 |  | C4H9O4 |
| C4H7O1-3OOH-4 | C1CC(O1)C(OO) | InChI=1S/C4H8O3/c5-7-3-4-1-2-6-4/h4-5H,1-3H2 |  | C4H8O3 |
| C4H7O1-3OOH-2 | C1C(OO)C(O1)C | InChI=1S/C4H8O3/c1-3-4(7-5)2-6-3/h3-5H,2H2,1H3 |  | C4H8O3 |
| C4H7O1-2OOH-4 | C1C(O1)CC(OO) | InChI=1S/C4H8O3/c5-7-2-1-4-3-6-4/h4-5H,1-3H2 |  | C4H8O3 |
| C4H7O1-4OOH-2 | C1C(OO)CC(O1) | InChI=1S/C4H8O3/c5-7-4-1-2-6-3-4/h4-5H,1-3H2 |  | C4H8O3 |
| C4H7O1-2OOH-3 | C1C(O1)C(OO)C | InChI=1S/C4H8O3/c1-3(7-5)4-2-6-4/h3-5H,2H2,1H3 | C4H8O3 |
| C4H7O2-3OOH-1 | C(OO)C1C(O1)C | InChI=1S/C4H8O3/c1-3-4(7-3)2-6-5/h3-5H,2H2,1H3 |  | C4H8O3 |
| HO2CH2CHO | C(COO)=O  | InChI=1S/C2H4O3/c3-1-2-5-4/h1,4H,2H2 |  | C2H4O3 |
| NC4KET12 | CCC(C=O)OO | InChI=1S/C4H8O3/c1-2-4(3-5)7-6/h3-4,6H,2H2,1H3 |  | C4H8O3 |
| NC4KET13 | CC(CC=O)OO | InChI=1S/C4H8O3/c1-4(7-6)2-3-5/h3-4,6H,2H2,1H3 |  | C4H8O3 |
| NC4KET14 | O=CCCCOO | InChI=1S/C4H8O3/c5-3-1-2-4-7-6/h3,6H,1-2,4H2 |  | C4H8O3 |
| NC4KET21 | CCC(=O)COO | InChI=1S/C4H8O3/c1-2-4(5)3-7-6/h6H,2-3H2,1H3 |  | C4H8O3 |
| NC4KET23 | CC(=O)C(C)OO | InChI=1S/C4H8O3/c1-3(5)4(2)7-6/h4,6H,1-2H3 |  | C4H8O3 |
| NC4KET24 | CC(=O)CCOO | InChI=1S/C4H8O3/c1-4(5)2-3-7-6/h6H,2-3H2,1H3 |  | C4H8O3 |
| C2H5COCH3 | CCC(C)=O | InChI=1S/C4H8O/c1-3-4(2)5/h3H2,1-2H3 |  | C4H8O |
| C2H5COCH2 | [CH2]C(=O)CC | InChI=1S/C4H7O/c1-3-4(2)5/h2-3H2,1H3 |  | C4H7O |
| CH2CH2COCH3 | [CH2]CC(C)=O | InChI=1S/C4H7O/c1-3-4(2)5/h1,3H2,2H3 |  | C4H7O |
| CH3CHCOCH3 | C[CH]C(C)=O | InChI=1S/C4H7O/c1-3-4(2)5/h3H,1-2H3 |  | C4H7O |
| C2H3COCH3 | C=CC(C)=O | InChI=1S/C4H6O/c1-3-4(2)5/h3H,1H2,2H3 |  | C4H6O |
| CH3CHOOCOCH3 | CC(=O)C(C)O[O] | InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4H,1-2H3 |  | C4H7O3 |
| CH2CHOOHCOCH3 | [CH2]C(OO)C(C)=O | InChI=1S/C4H7O3/c1-3(5)4(2)7-6/h4,6H,2H2,1H3 |  | C4H7O3 |
| NC3H7CHO | CCCC=O | InChI=1S/C4H8O/c1-2-3-4-5/h4H,2-3H2,1H3 |  | C4H8O |
| NC3H7CO | CCC[C]=O | InChI=1S/C4H7O/c1-2-3-4-5/h2-3H2,1H3 |  | C4H7O |
| C3H6CHO-3 | CC[CH]C=O | InChI=1S/C4H7O/c1-2-3-4-5/h3-4H,2H2,1H3 |  | C4H7O |
| C3H6CHO-2 | C[CH]CC=O | InChI=1S/C4H7O/c1-2-3-4-5/h2,4H,3H2,1H3 |  | C4H7O |
| C3H6CHO-1 | [CH2]CCC=O | InChI=1S/C4H7O/c1-2-3-4-5/h4H,1-3H2 |  | C4H7O |
| C2H5CHCO | CCC=C=O | InChI=1S/C4H6O/c1-2-3-4-5/h3H,2H2,1H3 |  | C4H6O |
| SC3H5CHO | CC=CC=O | InChI=1S/C4H6O/c1-2-3-4-5/h2-4H,1H3 |  | C4H6O |
| SC3H5CO | CC=C[C]=O | InChI=1S/C4H5O/c1-2-3-4-5/h2-3H,1H3 |  | C4H5O |
| CH2CH2CHO | [CH2]CC=O | InChI=1S/C3H5O/c1-2-3-4/h3H,1-2H2 |  | C3H5O |
| C4H7O2-1 | CC=CC[O]  | InChI=1S/C4H7O/c1-2-3-4-5/h2-3H,4H2,1H3 |  | C4H7O |
| IC4H10 | CC(C)C | InChI=1S/C4H10/c1-4(2)3/h4H,1-3H3 |  | C4H10 |
| IC4H9 | [CH2]C(C)C | InChI=1S/C4H9/c1-4(2)3/h4H,1H2,2-3H3 |  | C4H9 |
| IC4H8 | C=C(C)C | InChI=1S/C4H8/c1-4(2)3/h1H2,2-3H3 |  | C4H8 |
| IC4H7 | [CH2]C(=C)C | InChI=1S/C4H7/c1-4(2)3/h1-2H2,3H3 |  | C4H7 |
| TC4H9 | C[C](C)C | InChI=1S/C4H9/c1-4(2)3/h1-3H3 |  | C4H9 |
| TC4H9O2 | CC(C)(C)O[O] | InChI=1S/C4H9O2/c1-4(2,3)6-5/h1-3H3 |  | C4H9O2 |
| IC4H7OOCH3 | C=C(C)COOC  | InChI=1S/C5H10O2/c1-5(2)4-7-6-3/h1,4H2,2-3H3 |  | C5H10O2 |
| IC4H7OOIC4H7 | CC(=C)COOCC(=C)C | InChI=1S/C8H14O2/c1-7(2)5-9-10-6-8(3)4/h1,3,5-6H2,2,4H3 |  | C8H14O2 |
| IC3H5OCH2 | C=C(C)O[CH2]  | InChI=1S/C4H7O/c1-4(2)5-3/h1,3H2,2H3 |  | C4H7O |
| IC4H7-I1 | [CH]=C(C)C  | InChI=1S/C4H7/c1-4(2)3/h1H,2-3H3 |  | C4H7 |
| IC4H8OH-IT | C[C](C)CO  | InChI=1S/C4H9O/c1-4(2)3-5/h5H,3H2,1-2H3 |  | C4H9O |
| IC4H8OH-TI | [CH2]C(C)(C)O  | InChI=1S/C4H9O/c1-4(2,3)5/h5H,1H2,2-3H3 |  | C4H9O |
| IQJC4H8OH | CC(C)(CO[O])O  | InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h5H,3H2,1-2H3 |  | C4H9O3 |
| IQC4H8OT | CC(C)(COO)[O]  | InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h6H,3H2,1-2H3 |  | C4H9O3 |
| TQJC4H8OH | CC(C)(CO)O[O]  | InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5H,3H2,1-2H3 |  | C4H9O3 |
| TQC4H8OI | CC(C)(C[O])OO  | InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h6H,3H2,1-2H3 |  | C4H9O3 |
| TQC4H7OHI | CC(C)([CH]O)OO  | InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h3,5-6H,1-2H3 |  | C4H9O3 |
| IC3H4CHO-A | C=C([CH2])C=O  | InChI=1S/C4H5O/c1-4(2)3-5/h3H,1-2H2 |  | C4H5O |
| QC4H7OHP | [CH2]C(C)(CO)OO  | InChI=1S/C4H9O3/c1-4(2,3-5)7-6/h5-6H,1,3H2,2H3 |  | C4H9O3 |
| IQC4H7OHT | [CH2]C(C)(COO)O  | InChI=1S/C4H9O3/c1-4(2,5)3-7-6/h5-6H,1,3H2,2H3 |  | C4H9O3 |
| SC4H7OH-IP | C=C(C)[CH]O  | InChI=1S/C4H7O/c1-4(2)3-5/h3,5H,1H2,2H3 |  | C4H7O |
| C2CY(COC)OH | CC1(C)C(O)O1  | InChI=1S/C4H8O2/c1-4(2)3(5)6-4/h3,5H,1-2H3 |  | C4H8O2 |
| CCY(CCO)COH | CC1(CO)CO1  | InChI=1S/C4H8O2/c1-4(2-5)3-6-4/h5H,2-3H2,1H3 |  | C4H8O2 |
| CCY(CCOC)OH | CC1(COC1)O  | InChI=1S/C4H8O2/c1-4(5)2-6-3-4/h5H,2-3H2,1H3 |  | C4H8O2 |
| IC3H6OHCHO | CC(C)(C=O)O  | InChI=1S/C4H8O2/c1-4(2,6)3-5/h3,6H,1-2H3 |  | C4H8O2 |
| CH3COCOOH | CC(COO)=O  | InChI=1S/C3H6O3/c1-3(4)2-6-5/h5H,2H2,1H3 |  | C3H6O3 |
| IC3H5COHQ | C=C(C)C(O)OO  | InChI=1S/C4H8O3/c1-3(2)4(5)7-6/h4-6H,1H2,2H3 |  | C4H8O3 |
| IC3H5Q | C=C(C)OO  | InChI=1S/C3H6O2/c1-3(2)5-4/h4H,1H2,2H3 |  | C3H6O2 |
| TQC4H7OHIO2 | CC(C)(C(O)O[O])OO  | InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5,7H,1-2H3 |  | C4H9O5 |
| TQC4H7OHIQ-I | CC(C)(C([O])OO)OO  | InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,6-7H,1-2H3 |  | C4H9O5 |
| TQC4H7OHIQ-P | [CH2]C(C)(C(O)OO)OO  | InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5-7H,1H2,2H3 |  | C4H9O5 |
| CH2CQCOHQ | C=C(OO)C(O)OO | InChI=1S/C3H6O5/c1-2(7-5)3(4)8-6/h3-6H,1H2 |  | C3H6O5 |
| COHQCYC(COC) | CC1(CO1)C(O)OO  | InChI=1S/C4H8O4/c1-4(2-7-4)3(5)8-6/h3,5-6H,2H2,1H3 |  | C4H8O4 |
| QCYC(CCOC)OH | CC1(COC1O)OO  | InChI=1S/C4H8O4/c1-4(8-6)2-7-3(4)5/h3,5-6H,2H2,1H3 |  | C4H8O4 |
| TQC4H7OHTO2 | CC(C)(C(O)OO)O[O]  | InChI=1S/C4H9O5/c1-4(2,9-7)3(5)8-6/h3,5-6H,1-2H3 |  | C4H9O5 |
| HOCOCQ(CH3)2 | CC(C)(C(=O)O)OO  | InChI=1S/C4H8O4/c1-4(2,8-7)3(5)6/h7H,1-2H3,(H,5,6) |  | C4H8O4 |
| IQC4H7OHTO2 | CC(COO)(CO[O])O  | InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h5-6H,2-3H2,1H3 |  | C4H9O5 |
| TC3H6OH | C[C](C)O | InChI=1S/C3H7O/c1-3(2)4/h4H,1-2H3 |  | C3H7O |
| IQC4H7OHTQ-P | [CH2]C(COO)(COO)O  | InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h5-7H,1-3H2 |  | C4H9O5 |
| IQC4H8OTQ-I | CC(COO)(COO)[O]  | InChI=1S/C4H9O5/c1-4(5,2-8-6)3-9-7/h6-7H,2-3H2,1H3 |  | C4H9O5 |
| CH2COHCH2OOH | C=C(COO)O  | InChI=1S/C3H6O3/c1-3(4)2-6-5/h4-5H,1-2H2 |  | C3H6O3 |
| IC4H6Q2-II | C=C(COO)COO  | InChI=1S/C4H8O4/c1-4(2-7-5)3-8-6/h5-6H,1-3H2 |  | C4H8O4 |
| CO(CH2OOH)2 | C(C(COO)=O)OO  | InChI=1S/C3H6O5/c4-3(1-7-5)2-8-6/h5-6H,1-2H2 |  | C3H6O5 |
| CHOC(CH3)OHCH2Q | CC(C=O)(COO)O  | InChI=1S/C4H8O4/c1-4(6,2-5)3-8-7/h2,6-7H,3H2,1H3 |  | C4H8O4 |
| CH3COCHO | CC(C=O)=O  | InChI=1S/C3H4O2/c1-3(5)2-4/h2H,1H3 |  | C3H4O2 |
| SC4H7OH-I | CC(C)=CO  | InChI=1S/C4H8O/c1-4(2)3-5/h3,5H,1-2H3 | C4H8O |
| CCYCCC | CC1CC1  | InChI=1S/C4H8/c1-4-2-3-4/h4H,2-3H2,1H3 |  | C4H8 |
| H15DE25DM | C=C(C)CCC(=C)C  | InChI=1S/C8H14/c1-7(2)5-6-8(3)4/h1,3,5-6H2,2,4H3 |  | C8H14 |
| H15DE25DM-S | C=C(C)[CH]CC(=C)C  | InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h5H,1,3,6H2,2,4H3 |  | C8H13 |
| H15DE25DM-A | C=C([CH2])CCC(=C)C  | InChI=1S/C8H13/c1-7(2)5-6-8(3)4/h1-3,5-6H2,4H3 |  | C8H13 |
| H15DE25DM-AO | C=C(C)CCC(=C)C[O]  | InChI=1S/C8H13O/c1-7(2)4-5-8(3)6-9/h1,3-6H2,2H3 |  | C8H13O |
| H15DE2M-T | C=[C]CCC(=C)C  | InChI=1S/C7H11/c1-4-5-6-7(2)3/h1-2,5-6H2,3H3 |  | C7H11 |
| H15DE25DM-SO | C=C(C)CC(C(=C)C)[O]  | InChI=1S/C8H13O/c1-6(2)5-8(9)7(3)4/h8H,1,3,5H2,2,4H3 |  | C8H13O |
| IC4H7CHO | C=C(C)CC=O  | InChI=1S/C5H8O/c1-5(2)3-4-6/h4H,1,3H2,2H3 |  | C5H8O |
| AC5H10 | CCC(=C)C  | InChI=1S/C5H10/c1-4-5(2)3/h2,4H2,1,3H3 |  | C5H10 |
| AC5H9-A2 | CCC(=C)[CH2]  | InChI=1S/C5H9/c1-4-5(2)3/h2-4H2,1H3 |  | C5H9 |
| IC4H7O2 | C=C(C)CO[O]  | InChI=1S/C4H7O2/c1-4(2)3-6-5/h1,3H2,2H3 |  | C4H7O2 |
| IC4H6OOH-I | C=C([CH2])COO  | InChI=1S/C4H7O2/c1-4(2)3-6-5/h5H,1-3H2 |  | C4H7O2 |
| C\*CYCCOC | C=C1COC1  | InChI=1S/C4H6O/c1-4-2-5-3-4/h1-3H2 |  | C4H6O |
| CCYCCOOC-T1 | C[C]1COOC1  | InChI=1S/C4H7O2/c1-4-2-5-6-3-4/h2-3H2,1H3 |  | C4H7O2 |
| CCYCCOOC-I2 | CC1[CH]OOC1  | InChI=1S/C4H7O2/c1-4-2-5-6-3-4/h2,4H,3H2,1H3 |  | C4H7O2 |
| CHOIC3H6O | CC(C=O)C[O]  | InChI=1S/C4H7O2/c1-4(2-5)3-6/h2,4H,3H2,1H3 |  | C4H7O2 |
| CCY(C2O)CO | CC1(C[O])CO1  | InChI=1S/C4H7O2/c1-4(2-5)3-6-4/h2-3H2,1H3 |  | C4H7O2 |
| CCYCCO-T1 | C[C]1C(O1) | InChI=1S/C3H5O/c1-3-2-4-3/h2H2,1H3 |  | C3H5O |
| C2CYCOOC-I1 | [CH2]C1(C)COO1  | InChI=1S/C4H7O2/c1-4(2)3-5-6-4/h1,3H2,2H3 |  | C4H7O2 |
| IC3H5OOCH2 | C=C(C)OO[CH2]  | InChI=1S/C4H7O2/c1-4(2)6-5-3/h1,3H2,2H3 |  | C4H7O2 |
| B2E3M1OJ | CC(C)=CC[O]  | InChI=1S/C5H9O/c1-5(2)3-4-6/h3H,4H2,1-2H3 |  | C5H9O |
| B13DE2M | C=CC(=C)C  | InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3 |  | C5H8 |
| AC5H9-D | [CH2]CC(=C)C  | InChI=1S/C5H9/c1-4-5(2)3/h1-2,4H2,3H3 |  | C5H9 |
| B13DE2MJ | C=CC(=C)[CH2]  | InChI=1S/C5H7/c1-4-5(2)3/h4H,1-3H2 |  | C5H7 |
| AC5H9-C | C[CH]C(=C)C  | InChI=1S/C5H9/c1-4-5(2)3/h4H,2H2,1,3H3 |  | C5H9 |
| CC5H9-A | C=CC([CH2])C  | InChI=1S/C5H9/c1-4-5(2)3/h4-5H,1-2H2,3H3 |  | C5H9 |
| AC5H9O-C | C=C(C)C(C)[O]  | InChI=1S/C5H9O/c1-4(2)5(3)6/h5H,1H2,2-3H3 |  | C5H9O |
| B2E2M1OJ | CC=C(C)C[O]  | InChI=1S/C5H9O/c1-3-5(2)4-6/h3H,4H2,1-2H3 |  | C5H9O |
| CC5H9O-B | C=CC(C)(C)[O]  | InChI=1S/C5H9O/c1-4-5(2,3)6/h4H,1H2,2-3H3 |  | C5H9O |
| B12DE3M | [CH2]=[C]=[C](C)C  | InChI=1S/C5H8/c1-4-5(2)3/h1H2,2-3H3 |  | C5H8 |
| CC5H9-B | C=C[C](C)C  | InChI=1S/C5H9/c1-4-5(2)3/h4H,1H2,2-3H3 |  | C5H9 |
| IC4H9O2 | CC(C)CO[O] | InChI=1S/C4H9O2/c1-4(2)3-6-5/h4H,3H2,1-2H3 |  | C4H9O2 |
| TC4H8O2H-I | [CH2]C(C)(C)OO | InChI=1S/C4H9O2/c1-4(2,3)6-5/h5H,1H2,2-3H3 |  | C4H9O2 |
| IC4H8O2H-I | [CH2]C(C)COO | InChI=1S/C4H9O2/c1-4(2)3-6-5/h4-5H,1,3H2,2H3 |  | C4H9O2 |
| IC4H8O2H-T | C[C](C)COO | InChI=1S/C4H9O2/c1-4(2)3-6-5/h5H,3H2,1-2H3 |  | C4H9O2 |
| IC4H8O | CC1(C)CO1 | InChI=1S/C4H8O/c1-4(2)3-5-4/h3H2,1-2H3 |  | C4H8O |
| CC4H8O | C1C(C)CO1 | InChI=1S/C4H8O/c1-4-2-5-3-4/h4H,2-3H2,1H3 |  | C4H8O |
| IC4H9O | CC(C)C[O] | InChI=1S/C4H9O/c1-4(2)3-5/h4H,3H2,1-2H3 |  | C4H9O |
| TC4H9O | CC(C)(C)[O] | InChI=1S/C4H9O/c1-4(2,3)5/h1-3H3 |  | C4H9O |
| IC4H9O2H | CC(C)COO | InChI=1S/C4H10O2/c1-4(2)3-6-5/h4-5H,3H2,1-2H3 |  | C4H10O2 |
| TC4H9O2H | CC(C)(C)OO | InChI=1S/C4H10O2/c1-4(2,3)6-5/h5H,1-3H3 |  | C4H10O2 |
| IC4H7O | C=C(C)C[O] | InChI=1S/C4H7O/c1-4(2)3-5/h1,3H2,2H3 |  | C4H7O |
| IC4H8OH | [CH2]C(C)CO | InChI=1S/C4H9O/c1-4(2)3-5/h4-5H,1,3H2,2H3 |  | C4H9O |
| IC3H7CHO | CC(C)C=O | InChI=1S/C4H8O/c1-4(2)3-5/h3-4H,1-2H3 |  | C4H8O |
| TC3H6CHO | C[C](C)C=O | InChI=1S/C4H7O/c1-4(2)3-5/h3H,1-2H3 |  | C4H7O |
| IC3H7CO | CC(C)[C]=O | InChI=1S/C4H7O/c1-4(2)3-5/h4H,1-2H3 |  | C4H7O |
| IC3H6CHO | [CH2]C(C)C=O | InChI=1S/C4H7O/c1-4(2)3-5/h3-4H,1H2,2H3 |  | C4H7O |
| TC4H8OOH-IO2 | CC(C)(CO[O])OO | InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h6H,3H2,1-2H3 |  | C4H9O4 |
| IC4H8OOH-IO2 | CC(CO[O])COO | InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h4-5H,2-3H2,1H3 |  | C4H9O4 |
| IC4H8OOH-TO2 | CC(C)(COO)O[O] | InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5H,3H2,1-2H3 |  | C4H9O4 |
| IC4KETII | CC(C=O)COO | InChI=1S/C4H8O3/c1-4(2-5)3-7-6/h2,4,6H,3H2,1H3 |  | C4H8O3 |
| IC4KETIT | CC(C)(C=O)OO | InChI=1S/C4H8O3/c1-4(2,3-5)7-6/h3,6H,1-2H3 |  | C4H8O3 |
| IC4H7OH | C=C(C)CO | InChI=1S/C4H8O/c1-4(2)3-5/h5H,1,3H2,2H3 |  | C4H8O |
| IC4H6OH | [CH2]C(=C)CO | InChI=1S/C4H7O/c1-4(2)3-5/h5H,1-3H2 |  | C4H7O |
| IC3H5CHO | C=C(C)C=O | InChI=1S/C4H6O/c1-4(2)3-5/h3H,1H2,2H3 |  | C4H6O |
| IC3H5CO | C=C(C)[C]=O | InChI=1S/C4H5O/c1-4(2)3-5/h1H2,2H3 |  | C4H5O |
| TC3H6OCHO | CC(C)([O])C=O | InChI=1S/C4H7O2/c1-4(2,6)3-5/h3H,1-2H3 |  | C4H7O2 |
| IC3H6CO | CC(C)=C=O | InChI=1S/C4H6O/c1-4(2)3-5/h1-2H3 |  | C4H6O |
| IC4H7OOH | C=C(C)COO | InChI=1S/C4H8O2/c1-4(2)3-6-5/h5H,1,3H2,2H3 |  | C4H8O2 |
| TC3H6OHCHO | CC(C)(O)C=O | InChI=1S/C4H8O2/c1-4(2,6)3-5/h3,6H,1-2H3 |  | C4H8O2 |
| C3H6OH2-1 | [CH2]C(O)C | InChI=1S/C3H7O/c1-3(2)4/h3-4H,1H2,2H3 |  | C3H7O |
| IC3H5OH | C=C(C)O | InChI=1S/C3H6O/c1-3(2)4/h4H,1H2,2H3 |  | C3H6O |
| TC3H6O2CHO | CC(C)(C=O)O[O] | InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3H,1-2H3 |  | C4H7O3 |
| TC3H6O2HCO | CC(C)([C]=O)OO | InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h6H,1-2H3 |  | C4H7O3 |
| IC3H5O2HCHO | [CH2]C(C)(C=O)OO | InChI=1S/C4H7O3/c1-4(2,3-5)7-6/h3,6H,1H2,2H3 |  | C4H7O3 |
| CH2CCH2OH | C=[C]CO | InChI=1S/C3H5O/c1-2-3-4/h4H,1,3H2 |  | C3H5O |
| TC4H8CHO | [CH2]C(C)(C)C=O | InChI=1S/C5H9O/c1-5(2,3)4-6/h4H,1H2,2-3H3 |  | C5H9O |
| O2C4H8CHO | CC(C)(C=O)CO[O] | InChI=1S/C5H9O3/c1-5(2,3-6)4-8-7/h3H,4H2,1-2H3 |  | C5H9O3 |
| O2HC4H8CO | CC(C)([C]=O)COO | InChI=1S/C5H9O3/c1-5(2,3-6)4-8-7/h7H,4H2,1-2H3 |  | C5H9O3 |
| C3H5OH | C=CCO | InChI=1S/C3H6O/c1-2-3-4/h2,4H,1,3H2 |  | C3H6O |
| TIC4H7Q2-I | [CH2]C(C)(COO)OO | InChI=1S/C4H9O4/c1-4(2,8-6)3-7-5/h5-6H,1,3H2,2H3 |  | C4H9O4 |
| IIC4H7Q2-T | C[C](COO)COO | InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h5-6H,2-3H2,1H3 |  | C4H9O4 |
| IIC4H7Q2-I | [CH2]C(COO)COO | InChI=1S/C4H9O4/c1-4(2-7-5)3-8-6/h4-6H,1-3H2 |  | C4H9O4 |
| CH2O2H | [CH2]OO | InChI=1S/CH3O2/c1-3-2/h2H,1H2 |  | CH3O2 |
| C4H4 | C#CC=C | InChI=1S/C4H4/c1-3-4-2/h1,4H,2H2 |  | C4H4 |
| C4H3-I | C#C[C]=C | InChI=1S/C4H3/c1-3-4-2/h1H,2H2 |  | C4H3 |
| C4H3-N | [CH]=CC#C | InChI=1S/C4H3/c1-3-4-2/h1-3H |  | C4H3 |
| C4H612 | C=C=CC | InChI=1S/C4H6/c1-3-4-2/h4H,1H2,2H3 |  | C4H6 |
| C4H2 | C#CC#C | InChI=1S/C4H2/c1-3-4-2/h1-2H |  | C4H2 |
| C4H5-I | C=[C]C=C | InChI=1S/C4H5/c1-3-4-2/h3H,1-2H2 | C4H5 |
| C4H5-N | [CH]=CC=C | InChI=1S/C4H5/c1-3-4-2/h1,3-4H,2H2 |  | C4H5 |
| CH2CHCHCHO | [CH2]C=CC=O | InChI=1S/C4H5O/c1-2-3-4-5/h2-4H,1H2 |  | C4H5O |
| C4H6O25 | C1C=CCO1 | InChI=1S/C4H6O/c1-2-4-5-3-1/h1-2H,3-4H2 |  | C4H6O |
| C2H3CHOCH2 | C=CC1CO1 | InChI=1S/C4H6O/c1-2-4-3-5-4/h2,4H,1,3H2 |  | C4H6O |
| C4H5-2 | CC#C[CH2] | InChI=1S/C4H5/c1-3-4-2/h1H2,2H3 |  | C4H5 |
| C4H6-2 | CC#CC | InChI=1S/C4H6/c1-3-4-2/h1-2H3 |  | C4H6 |
| C4H6O23 | C1OC=CC1 | InChI=1S/C4H6O/c1-2-4-5-3-1/h1,3H,2,4H2 |  | C4H6O |
| C4H4O | CC#CC=O | InChI=1S/C4H4O/c1-2-3-4-5/h4H,1H3 |  | C4H4O |
| H2C4O | C#CC1=C(O1) | InChI=1S/C4H2O/c1-2-4-3-5-4/h1,3H |  | C4H2O |
| C2H3OCH2 | C1C(O1)[CH2] | InChI=1S/C3H5O/c1-3-2-4-3/h3H,1-2H2 | C3H5O |
| C6H6 | C1=CC=CC=C1 | InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H |  | C6H6 |
| C\*CCJC\*C | C=C[CH]C=C | InChI=1S/C5H7/c1-3-5-4-2/h3-5H,1-2H2 |  | C5H7 |
| C6H5 | C1=[C]C=CC=C1 | InChI=1S/C6H5/c1-2-4-6-5-3-1/h1-5H |  | C6H5 |
| C6H2 | C#CC#CC#C | InChI=1S/C6H2/c1-3-5-6-4-2/h1-2H |  | C6H2 |
| C6H3 | C#C[C]=CC#C | InChI=1S/C6H3/c1-3-5-6-4-2/h1-2,5H | C6H3 |
| L-C6H4 | C#CC=CC#C | InChI=1S/C6H4/c1-3-5-6-4-2/h1-2,5-6H | C6H4 |
| C-C6H4 | C#CC#CC=C | InChI=1S/C6H4/c1-3-5-6-4-2/h1,4H,2H2 | C6H4 |
| C6H5O | C1([O])=CC=CC=C1 | InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-5H |  | C6H5O |
| C6H5OH | C1(O)=CC=CC=C1 | InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h1-5,7H |  | C6H6O |
| P-C6H4O2 | C1(=O)C=CC(=O)C=C1 | InChI=1S/C6H4O2/c7-5-1-2-6(8)4-3-5/h1-4H |  | C6H4O2 |
| O-C6H4O2 | C1(=O)C(=O)C=CC=C1 | InChI=1S/C6H4O2/c7-5-3-1-2-4-6(5)8/h1-4H | C6H4O2 |
| P-C6H3O2 | C1(=O)[C]=CC(=O)C=C1 | InChI=1S/C6H3O2/c7-5-1-2-6(8)4-3-5/h1-3H |  | C6H3O2 |
| C5H6 | C1C=CC=C1 | InChI=1S/C5H6/c1-2-4-5-3-1/h1-4H,5H2 | C5H6 |
| C5H5 | [CH]1C=CC=C1 | InChI=1S/C5H5/c1-2-4-5-3-1/h1-5H |  | C5H5 |
| C5H4O | C1(=O)C=CC=C1 | InChI=1S/C5H4O/c6-5-3-1-2-4-5/h1-4H |  | C5H4O |
| C5H5O | C1([O])C=CC=C1 | InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1-5H |  | C5H5O |
| C5H5OH | C1(O)C=CC=C1 | InChI=1S/C5H6O/c6-5-3-1-2-4-5/h1-6H |  | C5H6O |
| C5H4OH | [C](O)1C=CC=C1 | InChI=1S/C5H5O/c6-5-3-1-2-4-5/h1-4,6H |  | C5H5O |
| C5H3O | C1(=O)[C]=CC=C1 | InChI=1S/C5H3O/c6-5-3-1-2-4-5/h1-3H |  | C5H3O |
| C6H5OO | C1=C(O[O])C=CC=C1 | InChI=1S/C6H5O2/c7-8-6-4-2-1-3-5-6/h1-5H |  | C6H5O2 |
| C6H5OOH | C1=C(OO)C=CC=C1 | InChI=1S/C6H6O2/c7-8-6-4-2-1-3-5-6/h1-5,7H |  | C6H6O2 |
| OC6H4OH | C1=C([O])C=C(O)C=C1 | InChI=1S/C6H5O2/c7-5-2-1-3-6(8)4-5/h1-4,7H |  | C6H5O2 |
| C6H4OH | C1=[C]C=C(O)C=C1 | InChI=1S/C6H5O/c7-6-4-2-1-3-5-6/h1-2,4-5,7H |  | C6H5O |
| O-OC6H5OJ | C1(=O)C([O])C=CC=C1 | InChI=1S/C6H5O2/c7-5-3-1-2-4-6(5)8/h1-5H |  | C6H5O2 |
| P-OC6H5OJ | C1(=O)C=CC([O])C=C1 | InChI=1S/C6H5O2/c7-5-1-2-6(8)4-3-5/h1-5H |  | C6H5O2 |
| C#CC\*CCJ | C#CC=C[CH2] | InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2 | C5H5 |
| C5H6-L | C#CC=CC | InChI=1S/C5H6/c1-3-5-4-2/h1,4-5H,2H3 |  | C5H6 |
| CJ\*CC\*CC\*O | [CH]=CC=CC=O | InChI=1S/C5H5O/c1-2-3-4-5-6/h1-5H |  | C5H5O |
| C\*CC\*CCJ\*O | C=CC=C[C]=O | InChI=1S/C5H5O/c1-2-3-4-5-6/h2-4H,1H2 |  | C5H5O |
| CJ\*CC\*O | [CH]=CC=CC=O | InChI=1S/C5H5O/c1-2-3-4-5-6/h1-5H |  | C5H5O |
| C5H7 | C1C[CH]C=C1 | InChI=1S/C5H7/c1-2-4-5-3-1/h1-3H,4-5H2 |  | C5H7 |
| OC5H7O | C(=O)[CH]CCC(=O) | InChI=1S/C5H7O2/c6-4-2-1-3-5-7/h2,4-5H,1,3H2 |  | C5H7O2 |
| C\*CCJC\*COH | C=C[CH]C=C(O) | InChI=1S/C5H7O/c1-2-3-4-5-6/h2-6H,1H2 |  | C5H7O |
| C\*CC\*CCJ | C#CC=C[CH2] | InChI=1S/C5H5/c1-3-5-4-2/h1,4-5H,2H2 |  | C5H5 |
| C\*CC\*CCOH | C=CC=CC(O) | InChI=1S/C5H8O/c1-2-3-4-5-6/h2-4,6H,1,5H2 |  | C5H8O |
| C5H81-3 | C=CC=CC  | InChI=1S/C5H8/c1-3-5-4-2/h3-5H,1H2,2H3 |  | C5H8 |
| OC4H6O | C(=O)CCC(=O) | InChI=1S/C4H6O2/c5-3-1-2-4-6/h3-4H,1-2H2 |  | C4H6O2 |
| OC4H5O | C(=O)CC[C](=O) | InChI=1S/C4H5O2/c5-3-1-2-4-6/h3H,1-2H2 |  | C4H5O2 |
| HOCO | [C](=O)O | InChI=1S/CHO2/c2-1-3/h(H,2,3) |  | CHO2 |
| HOC\*CC\*O | C(O)=CC=O | InChI=1S/C3H4O2/c4-2-1-3-5/h1-4H |  | C3H4O2 |
| HOC\*CCJ\*O | C(O)=C[C]=O | InChI=1S/C3H3O2/c4-2-1-3-5/h1-2,4H |  | C3H3O2 |
| O2CCHOOJ | C(=O)(O)C(=O)[O] | InChI=1S/C2HO4/c3-1(4)2(5)6/h(H,3,4) |  | C2HO4 |
| C6H101-5 | C=CCCC=C | InChI=1S/C6H10/c1-3-5-6-4-2/h3-4H,1-2,5-6H2 | C6H10 |
| C6H9-A | C=CC[CH]C=C | InChI=1S/C6H9/c1-3-5-6-4-2/h3-5H,1-2,6H2 |  | C6H9 |
| C3H2 | C=C=[C] | InChI=1S/C3H2/c1-3-2/H1h2 | C:\Users\0116383s\AppData\Local\Temp\mx3383D.png | C3H2 |
| C3H2(S) | C=C=[C] | InChI=1S/C3H2/c1-3-2/H1h2 | C:\Users\0116383s\AppData\Local\Temp\mx3383D.png | C3H2 |
| C3H2C | C1=C[C]1 | InChI=1S/C3H2/c1-2-3-1/h1-2H | C:\Users\0116383s\AppData\Local\Temp\mx3648A.png | C3H2 |
| H2CCC(S) | C=C=[C] | InChI=1S/C3H2/c1-3-2/H1h2 | C:\Users\0116383s\AppData\Local\Temp\mx3383D.png | C3H2 |
| C3H3O | C=C=C([O]) | InChI=1S/C3H3O/c1-2-3-4/h3H,1H2 |  | C3H3O |
| C3H3O2H | C=C=C(OO) | InChI=1S/C3H4O2/c1-2-3-5-4/h3-4H,1H2 |  | C3H4O2 |
| C2HCHO | C#CC=O | InChI=1S/C3H2O/c1-2-3-4/h1,3H |  | C3H2O |
| CH3COCH2O | CC(=O)C[O] | InChI=1S/C3H5O2/c1-3(5)2-4/h2H2,1H3 | C3H5O2 |
| PC3H4OH-2 | C[C]=CO  | InChI=1S/C3H5O/c1-2-3-4/h3-4H,1H3 |  | C3H5O |
| SC3H4OH | C=C([CH2])O  | InChI=1S/C3H5O/c1-3(2)4/h4H,1-2H2 |  | C3H5O |
| SC3H5OH | CC=CO  | InChI=1S/C3H6O/c1-2-3-4/h2-4H,1H3 |  | C3H6O |
| CH3CHCHO | C[CH]C=O | InChI=1S/C3H5O/c1-2-3-4/h2-3H,1H3 |  | C3H5O |
| AC4H7OOH | C=CCOOC  | InChI=1S/C4H8O2/c1-3-4-6-5-2/h3H,1,4H2,2H3 |  | C4H8O2 |
| TQJC3H6OH | C(O)C(O[O])C | InChI=1S/C3H7O3/c1-3(2-4)6-5/h3-4H,2H2,1H3 |  | C3H7O3 |
| TQC3H6OI | CC(OO)C([O]) | InChI=1S/C3H7O3/c1-3(2-4)6-5/h3,5H,2H2,1H3 |  | C3H7O3 |
| QC3H5OHP | C(O)C(OO)[CH2] | InChI=1S/C3H7O3/c1-3(2-4)6-5/h3-5H,1-2H2 |  | C3H7O3 |
| TQC3H5OHI | [CH](O)C(OO)C | InChI=1S/C3H7O3/c1-3(2-4)6-5/h2-5H,1H3 |  | C3H7O3 |
| CCY(COC)OH | CC1C(O)O1 | InChI=1S/C3H6O2/c1-2-3(4)5-2/h2-4H,1H3 |  | C3H6O2 |
| IQJC3H6OH | C(O[O])C(O)C | InChI=1S/C3H7O3/c1-3(4)2-6-5/h3-4H,2H2,1H3 |  | C3H7O3 |
| IQC3H6OT | C(OO)C([O])C | InChI=1S/C3H7O3/c1-3(4)2-6-5/h3,5H,2H2,1H3 |  | C3H7O3 |
| IQC3H5OHPJ | C(OO)C(O)[CH2] | InChI=1S/C3H7O3/c1-3(4)2-6-5/h3-5H,1-2H2 |  | C3H7O3 |
| CHOCH2OOH | C(=O)COO | InChI=1S/C2H4O3/c3-1-2-5-4/h1,4H,2H2 |  | C2H4O3 |
| CY(CCOC)OH | C1C(O)CO1 | InChI=1S/C3H6O2/c4-3-1-5-2-3/h3-4H,1-2H2 |  | C3H6O2 |
| CHOCOHCH3 | C(=O)C(O)C | InChI=1S/C3H6O2/c1-3(5)2-4/h2-3,5H,1H3 |  | C3H6O2 |
| CY(COC)COH | C1C(O1)C(O) | InChI=1S/C3H6O2/c4-1-3-2-5-3/h3-4H,1-2H2 |  | C3H6O2 |
| TQC3H5OHIO2 | C(O)(O[O])C(OO)C | InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h2-5H,1H3 |  | C3H7O5 |
| TQC3H5OHIQ-I | C([O])(OO)C(OO)C | InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h2-3,5-6H,1H3 |  | C3H7O5 |
| TQC3H5OHIQ-P | C(O)(OO)C(OO)[CH2] | InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h2-6H,1H2 |  | C3H7O5 |
| C2H3COHOOH | C=CC(O)(OO) | InChI=1S/C3H6O3/c1-2-3(4)6-5/h2-5H,1H2 |  | C3H6O3 |
| COHOOHCY(COC) | C1C(O1)C(O)(OO) | InChI=1S/C3H6O4/c4-3(7-5)2-1-6-2/h2-5H,1H2 |  | C3H6O4 |
| OHCY(COCC)OOH | C1C(OO)C(O)O1 | InChI=1S/C3H6O4/c4-3-2(7-5)1-6-3/h2-5H,1H2 | C3H6O4 |
| IQC3H5OHPJO2 | C(OO)C(O)C(O[O]) | InChI=1S/C3H7O5/c4-3(1-7-5)2-8-6/h3-5H,1-2H2 |  | C3H7O5 |
| IQC3H5OTQ-I | C(OO)C([O])C(OO) | InChI=1S/C3H7O5/c4-3(1-7-5)2-8-6/h3,5-6H,1-2H2 |  | C3H7O5 |
| IQC3H5OHQ-SJ | [CH](OO)C(O)C(OO) | InChI=1S/C3H7O5/c4-3(1-7-5)2-8-6/h1,3-6H,2H2 |  | C3H7O5 |
| CHOCOHCH2OOH | C(=O)C(O)C(OO) | InChI=1S/C3H6O4/c4-1-3(5)2-7-6/h1,3,5-6H,2H2 |  | C3H6O4 |
| CHOCHO | O=CC=O | InChI=1S/C2H2O2/c3-1-2-4/h1-2H | C2H2O2 |
| TQC3H5OHTO2 | C(O)(OO)C(O[O])C | InChI=1S/C3H7O5/c1-2(7-5)3(4)8-6/h2-4,6H,1H3 |  | C3H7O5 |
| OHCOCOOHCH3 | C(O)(=O)C(OO)C | InChI=1S/C3H6O4/c1-2(7-6)3(4)5/h2,6H,1H3,(H,4,5) |  | C3H6O4 |
| C2H3OO | C=C(O[O]) | InChI=1S/C2H3O2/c1-2-4-3/h2H,1H2 |  | C2H3O2 |
| CHCHO | [CH]C=O | InChI=1S/C2H2O/c1-2-3/h1-2H | C:\Users\0116383s\AppData\Local\Temp\mx3BC9E.png | C2H2O |
| C4H71-3OH | C=CC(O)C | InChI=1S/C4H8O/c1-3-4(2)5/h3-5H,1H2,2H3 |  | C4H8O |
| C4H71-1OH | C(O)=CCC | InChI=1S/C4H8O/c1-2-3-4-5/h3-5H,2H2,1H3 |  | C4H8O |
| C4H71-2OH | C=C(O)CC | InChI=1S/C4H8O/c1-3-4(2)5/h5H,2-3H2,1H3 |  | C4H8O |
| PC4H8OH-2 | C(O)[CH]CC | InChI=1S/C4H9O/c1-2-3-4-5/h3,5H,2,4H2,1H3 |  | C4H9O |
| SC4H8OH-1 | [CH2]C(O)CC | InChI=1S/C4H9O/c1-3-4(2)5/h4-5H,2-3H2,1H3 |  | C4H9O |
| C-2-C4H8 | CC=CC | InChI=1S/C4H8/c1-3-4-2/h3-4H,1-2H3/b4-3- | C:\Users\0116383s\AppData\Local\Temp\mx38D2F.png | C4H8 |
| C4H6-1 | C#CCC | InChI=1S/C4H6/c1-3-4-2/h1H,4H2,2H3 |  | C4H6 |
| C3H5OCH2-1 | C=CCO[CH2] | InChI=1S/C4H7O/c1-3-4-5-2/h3H,1-2,4H2 |  | C4H7O |
| NC5H12 | CCCCC  | InChI=1S/C5H12/c1-3-5-4-2/h3-5H2,1-2H3 |  | C5H12 |
| C5H11-1 | [CH2]CCCC  | InChI=1S/C5H11/c1-3-5-4-2/h1,3-5H2,2H3 |  | C5H11 |
| C5H11-2 | C[CH]CCC  | InChI=1S/C5H11/c1-3-5-4-2/h3H,4-5H2,1-2H3 |  | C5H11 |
| C5H11-3 | CC[CH]CC  | InChI=1S/C5H11/c1-3-5-4-2/h5H,3-4H2,1-2H3 |  | C5H11 |
| C5H10-1 | C=CCCC  | InChI=1S/C5H10/c1-3-5-4-2/h3H,1,4-5H2,2H3 |  | C5H10 |
| C5H10-2 | CC=CCC  | InChI=1S/C5H10/c1-3-5-4-2/h3,5H,4H2,1-2H3 |  | C5H10 |
| C5H91-3 | C=C[CH]CC  | InChI=1S/C5H9/c1-3-5-4-2/h3,5H,1,4H2,2H3 |  | C5H9 |
| C5H91-4 | C=CC[CH]C  | InChI=1S/C5H9/c1-3-5-4-2/h3-4H,1,5H2,2H3 |  | C5H9 |
| C5H91-5 | C=CCC[CH2]  | InChI=1S/C5H9/c1-3-5-4-2/h3H,1-2,4-5H2 |  | C5H9 |
| C5H92-4 | CC=C[CH]C  | InChI=1S/C5H9/c1-3-5-4-2/h3-5H,1-2H3 |  | C5H9 |
| C5H92-5 | [CH2]CC=CC  | InChI=1S/C5H9/c1-3-5-4-2/h4-5H,1,3H2,2H3 |  | C5H9 |
| C5H9O1-3 | C=CC(CC)[O]  | InChI=1S/C5H9O/c1-3-5(6)4-2/h3,5H,1,4H2,2H3 |  | C5H9O |
| C5H9O2-4 | CC=CC(C)[O]  | InChI=1S/C5H9O/c1-3-4-5(2)6/h3-5H,1-2H3 |  | C5H9O |
| C5H11O2H-1 | CCCCCOO  | InChI=1S/C5H12O2/c1-2-3-4-5-7-6/h6H,2-5H2,1H3 |  | C5H12O2 |
| C5H11O2H-2 | CCCC(C)OO  | InChI=1S/C5H12O2/c1-3-4-5(2)7-6/h5-6H,3-4H2,1-2H3 |  | C5H12O2 |
| C5H11O2H-3 | CCC(CC)OO  | InChI=1S/C5H12O2/c1-3-5(4-2)7-6/h5-6H,3-4H2,1-2H3 |  | C5H12O2 |
| C5H11O2-1 | CCCCCO[O]  | InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h2-5H2,1H3 |  | C5H11O2 |
| C5H11O2-2 | CCCC(C)O[O]  | InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5H,3-4H2,1-2H3 |  | C5H11O2 |
| C5H11O2-3 | CCC(CC)O[O]  | InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h5H,3-4H2,1-2H3 |  | C5H11O2 |
| C5H11O-1 | CCCCC[O]  | InChI=1S/C5H11O/c1-2-3-4-5-6/h2-5H2,1H3 |  | C5H11O |
| C5H11O-2 | CCCC(C)[O]  | InChI=1S/C5H11O/c1-3-4-5(2)6/h5H,3-4H2,1-2H3 |  | C5H11O |
| C5H11O-3 | CCC(CC)[O]  | InChI=1S/C5H11O/c1-3-5(6)4-2/h5H,3-4H2,1-2H3 |  | C5H11O |
| C5H10OOH1-2 | CCC[CH]COO  | InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h4,6H,2-3,5H2,1H3 |  | C5H11O2 |
| C5H10OOH1-3 | CC[CH]CCOO  | InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h3,6H,2,4-5H2,1H3 |  | C5H11O2 |
| C5H10OOH1-4 | C[CH]CCCOO  | InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h2,6H,3-5H2,1H3 |  | C5H11O2 |
| C5H10OOH1-5 | [CH2]CCCCOO  | InChI=1S/C5H11O2/c1-2-3-4-5-7-6/h6H,1-5H2 |  | C5H11O2 |
| C5H10OOH2-1 | CCCC([CH2])OO  | InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5-6H,2-4H2,1H3 |  | C5H11O2 |
| C5H10OOH2-3 | CC[CH]C(C)OO  | InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h4-6H,3H2,1-2H3 |  | C5H11O2 |
| C5H10OOH2-4 | C[CH]CC(C)OO  | InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h3,5-6H,4H2,1-2H3 |  | C5H11O2 |
| C5H10OOH2-5 | [CH2]CCC(C)OO  | InChI=1S/C5H11O2/c1-3-4-5(2)7-6/h5-6H,1,3-4H2,2H3 |  | C5H11O2 |
| C5H10OOH3-1 | [CH2]CC(CC)OO  | InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h5-6H,1,3-4H2,2H3 |  | C5H11O2 |
| C5H10OOH3-2 | C[CH]C(CC)OO  | InChI=1S/C5H11O2/c1-3-5(4-2)7-6/h3,5-6H,4H2,1-2H3 |  | C5H11O2 |
| C5H10O1-2 | CCCC1CO1  | InChI=1S/C5H10O/c1-2-3-5-4-6-5/h5H,2-4H2,1H3 |  | C5H10O |
| C5H10O1-3 | CCC1CCO1  | InChI=1S/C5H10O/c1-2-5-3-4-6-5/h5H,2-4H2,1H3 |  | C5H10O |
| C5H10O1-4 | CC1CCCO1  | InChI=1S/C5H10O/c1-5-3-2-4-6-5/h5H,2-4H2,1H3 |  | C5H10O |
| C5H10O1-5 | C1CCOCC1  | InChI=1S/C5H10O/c1-2-4-6-5-3-1/h1-5H2 |  | C5H10O |
| C5H10O2-3 | CCC1C(C)O1  | InChI=1S/C5H10O/c1-3-5-4(2)6-5/h4-5H,3H2,1-2H3 |  | C5H10O |
| C5H10O2-4 | CC1CC(C)O1  | InChI=1S/C5H10O/c1-4-3-5(2)6-4/h4-5H,3H2,1-2H3 |  | C5H10O |
| C5H10OOH1-2O2 | CCCC(COO)O[O]  | InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5-6H,2-4H2,1H3 |  | C5H11O4 |
| C5H10OOH1-3O2 | CCC(CCOO)O[O]  | InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5-6H,2-4H2,1H3 |  | C5H11O4 |
| C5H10OOH1-4O2 | CC(CCCOO)O[O]  | InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5-6H,2-4H2,1H3 |  | C5H11O4 |
| C5H10OOH1-5O2 | C(CCOO)CCO[O]  | InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h6H,1-5H2 |  | C5H11O4 |
| C5H10OOH2-1O2 | CCCC(CO[O])OO  | InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5,7H,2-4H2,1H3 |  | C5H11O4 |
| C5H10OOH2-3O2 | CCC(C(C)OO)O[O]  | InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-6H,3H2,1-2H3 |  | C5H11O4 |
| C5H10OOH2-4O2 | CC(CC(C)O[O])OO  | InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h4-6H,3H2,1-2H3 |  | C5H11O4 |
| C5H10OOH2-5O2 | CC(CCCO[O])OO  | InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5,7H,2-4H2,1H3 |  | C5H11O4 |
| C5H10OOH3-1O2 | CCC(CCO[O])OO  | InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5,7H,2-4H2,1H3 |  | C5H11O4 |
| C5H10OOH3-2O2 | CCC(C(C)O[O])OO  | InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-5,7H,3H2,1-2H3 |  | C5H11O4 |
| C5H91-2,3OOH | CCC(C([CH2])OO)OO  | InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-7H,2-3H2,1H3 |  | C5H11O4 |
| C5H91-2,4OOH | [CH2]C(CC(C)OO)OO  | InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h4-7H,1,3H2,2H3 |  | C5H11O4 |
| C5H91-2,5OOH | [CH2]C(CCCOO)OO  | InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h5-7H,1-4H2 |  | C5H11O4 |
| C5H91-3,4OOH | [CH2]CC(C(C)OO)OO  | InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h4-7H,1,3H2,2H3 |  | C5H11O4 |
| C5H91-3,5OOH | [CH2]CC(CCOO)OO  | InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h5-7H,1-4H2 |  | C5H11O4 |
| C5H91-4,5OOH | [CH2]CCC(COO)OO  | InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h5-7H,1-4H2 |  | C5H11O4 |
| C5H92-1,3OOH | CCC([CH]COO)OO  | InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h3,5-7H,2,4H2,1H3 |  | C5H11O4 |
| C5H92-1,4OOH | CC(C[CH]COO)OO  | InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h2,5-7H,3-4H2,1H3 |  | C5H11O4 |
| C5H92-1,5OOH | C([CH]COO)CCOO  | InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h2,6-7H,1,3-5H2 |  | C5H11O4 |
| C5H92-3,4OOH | C[CH]C(C(C)OO)OO  | InChI=1S/C5H11O4/c1-3-5(9-7)4(2)8-6/h3-7H,1-2H3 |  | C5H11O4 |
| C5H92-3,5OOH | C[CH]C(CCOO)OO  | InChI=1S/C5H11O4/c1-2-5(9-7)3-4-8-6/h2,5-7H,3-4H2,1H3 |  | C5H11O4 |
| C5H92-4,5OOH | C[CH]CC(COO)OO  | InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h2,5-7H,3-4H2,1H3 |  | C5H11O4 |
| C5H93-1,2OOH | CC[CH]C(COO)OO  | InChI=1S/C5H11O4/c1-2-3-5(9-7)4-8-6/h3,5-7H,2,4H2,1H3 |  | C5H11O4 |
| C5H93-1,4OOH | CC([CH]CCOO)OO  | InChI=1S/C5H11O4/c1-5(9-7)3-2-4-8-6/h3,5-7H,2,4H2,1H3 |  | C5H11O4 |
| C5H93-1,5OOH | [CH](CCOO)CCOO  | InChI=1S/C5H11O4/c6-8-4-2-1-3-5-9-7/h1,6-7H,2-5H2 |  | C5H11O4 |
| C5H93-2,4OOH | CC([CH]C(C)OO)OO  | InChI=1S/C5H11O4/c1-4(8-6)3-5(2)9-7/h3-7H,1-2H3 |  | C5H11O4 |
| C5H91-3OOH | C=CC(CC)OO  | InChI=1S/C5H10O2/c1-3-5(4-2)7-6/h3,5-6H,1,4H2,2H3 |  | C5H10O2 |
| C5H91-4OOH | C=CCC(C)OO  | InChI=1S/C5H10O2/c1-3-4-5(2)7-6/h3,5-6H,1,4H2,2H3 |  | C5H10O2 |
| C5H91-5OOH | C=CCCCOO  | InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h2,6H,1,3-5H2 |  | C5H10O2 |
| C5H92-1OOH | CCC=CCOO  | InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h3-4,6H,2,5H2,1H3 |  | C5H10O2 |
| C5H92-4OOH | CC=CC(C)OO  | InChI=1S/C5H10O2/c1-3-4-5(2)7-6/h3-6H,1-2H3 |  | C5H10O2 |
| C5H92-5OOH | CC=CCCOO  | InChI=1S/C5H10O2/c1-2-3-4-5-7-6/h2-3,6H,4-5H2,1H3 |  | C5H10O2 |
| C5H9O1-2OOH-3 | CCC(C1CO1)OO  | InChI=1S/C5H10O3/c1-2-4(8-6)5-3-7-5/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O1-2OOH-4 | CC(CC1CO1)OO  | InChI=1S/C5H10O3/c1-4(8-6)2-5-3-7-5/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O1-2OOH-5 | C(CC1CO1)COO  | InChI=1S/C5H10O3/c6-8-3-1-2-5-4-7-5/h5-6H,1-4H2 |  | C5H10O3 |
| C5H9O1-3OOH-2 | CCC1C(CO1)OO  | InChI=1S/C5H10O3/c1-2-4-5(8-6)3-7-4/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O1-3OOH-4 | CC(C1CCO1)OO  | InChI=1S/C5H10O3/c1-4(8-6)5-2-3-7-5/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O1-3OOH-5 | C1COC1CCOO  | InChI=1S/C5H10O3/c6-8-4-2-5-1-3-7-5/h5-6H,1-4H2 |  | C5H10O3 |
| C5H9O1-4OOH-2 | CC1CC(CO1)OO  | InChI=1S/C5H10O3/c1-4-2-5(8-6)3-7-4/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O1-4OOH-3 | CC1C(CCO1)OO  | InChI=1S/C5H10O3/c1-4-5(8-6)2-3-7-4/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O1-4OOH-5 | C1CC(COO)OC1  | InChI=1S/C5H10O3/c6-8-4-5-2-1-3-7-5/h5-6H,1-4H2 |  | C5H10O3 |
| C5H9O1-5OOH-2 | C1CC(COC1)OO  | InChI=1S/C5H10O3/c6-8-5-2-1-3-7-4-5/h5-6H,1-4H2 |  | C5H10O3 |
| C5H9O1-5OOH-3 | C1COCCC1OO  | InChI=1S/C5H10O3/c6-8-5-1-3-7-4-2-5/h5-6H,1-4H2 |  | C5H10O3 |
| C5H9O2-3OOH-1 | CCC1C(COO)O1  | InChI=1S/C5H10O3/c1-2-4-5(8-4)3-7-6/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O2-3OOH-4 | CC1C(C(C)OO)O1  | InChI=1S/C5H10O3/c1-3-5(7-3)4(2)8-6/h3-6H,1-2H3 |  | C5H10O3 |
| C5H9O2-3OOH-5 | CC1C(CCOO)O1  | InChI=1S/C5H10O3/c1-4-5(8-4)2-3-7-6/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O2-4OOH-1 | CC1CC(COO)O1  | InChI=1S/C5H10O3/c1-4-2-5(8-4)3-7-6/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9O2-4OOH-3 | CC1C(C(C)O1)OO  | InChI=1S/C5H10O3/c1-3-5(8-6)4(2)7-3/h3-6H,1-2H3 |  | C5H10O3 |
| OCH2CHO | C(C[O])=O  | InChI=1S/C2H3O2/c3-1-2-4/h1H,2H2 |  | C2H3O2 |
| C5H9O1-2O-5 | C(CC1CO1)C[O]  | InChI=1S/C5H9O2/c6-3-1-2-5-4-7-5/h5H,1-4H2 |  | C5H9O2 |
| CH2OCH2CHO | [CH2]OCC=O  | InChI=1S/C3H5O2/c1-5-3-2-4/h2H,1,3H2 |  | C3H5O2 |
| C2H4OCHO | CC(C=O)[O]  | InChI=1S/C3H5O2/c1-3(5)2-4/h2-3H,1H3 |  | C3H5O2 |
| CH2CH2OCH2CH2CHO | [CH2]COCCC=O  | InChI=1S/C5H9O2/c1-2-7-5-3-4-6/h4H,1-3,5H2 | C5H9O2 |
| C4H7O1-4 | C=CCC[O]  | InChI=1S/C4H7O/c1-2-3-4-5/h2H,1,3-4H2 |  | C4H7O |
| NC5KET12 | CCCC(C=O)OO  | InChI=1S/C5H10O3/c1-2-3-5(4-6)8-7/h4-5,7H,2-3H2,1H3 |  | C5H10O3 |
| NC5KET13 | CCC(CC=O)OO  | InChI=1S/C5H10O3/c1-2-5(8-7)3-4-6/h4-5,7H,2-3H2,1H3 | C5H10O3 |
| NC5KET14 | CC(CCC=O)OO  | InChI=1S/C5H10O3/c1-5(8-7)3-2-4-6/h4-5,7H,2-3H2,1H3 |  | C5H10O3 |
| NC5KET15 | C(CC=O)CCOO  | InChI=1S/C5H10O3/c6-4-2-1-3-5-8-7/h4,7H,1-3,5H2 |  | C5H10O3 |
| NC5KET21 | CCCC(COO)=O  | InChI=1S/C5H10O3/c1-2-3-5(6)4-8-7/h7H,2-4H2,1H3 |  | C5H10O3 |
| NC5KET23 | CCC(C(C)=O)OO  | InChI=1S/C5H10O3/c1-3-5(8-7)4(2)6/h5,7H,3H2,1-2H3 |  | C5H10O3 |
| NC5KET24 | CC(CC(C)OO)=O  | InChI=1S/C5H10O3/c1-4(6)3-5(2)8-7/h5,7H,3H2,1-2H3 |  | C5H10O3 |
| NC5KET25 | CC(CCCOO)=O  | InChI=1S/C5H10O3/c1-5(6)3-2-4-8-7/h7H,2-4H2,1H3 |  | C5H10O3 |
| NC5KET31 | CCC(CCOO)=O  | InChI=1S/C5H10O3/c1-2-5(6)3-4-8-7/h7H,2-4H2,1H3 |  | C5H10O3 |
| NC5KET32 | CCC(C(C)OO)=O  | InChI=1S/C5H10O3/c1-3-5(6)4(2)8-7/h4,7H,3H2,1-2H3 |  | C5H10O3 |
| CHOC4H8O | CCCC(C=O)[O]  | InChI=1S/C5H9O2/c1-2-3-5(7)4-6/h4-5H,2-3H2,1H3 |  | C5H9O2 |
| CHOCH2CH2C2H4O | CC(CCC=O)[O]  | InChI=1S/C5H9O2/c1-5(7)3-2-4-6/h4-5H,2-3H2,1H3 | C5H9O2 |
| CHOCH2CH2CH2CH2O | C(CC=O)CC[O]  | InChI=1S/C5H9O2/c6-4-2-1-3-5-7/h4H,1-3,5H2 | C5H9O2 |
| C3H7COCH2O | CCCC(C[O])=O  | InChI=1S/C5H9O2/c1-2-3-5(7)4-6/h2-4H2,1H3 |  | C5H9O2 |
| CH3COC3H6O | CCC(C(C)=O)[O]  | InChI=1S/C5H9O2/c1-3-5(7)4(2)6/h5H,3H2,1-2H3 |  | C5H9O2 |
| CH3COCH2CH2CH2O | CC(CCC[O])=O  | InChI=1S/C5H9O2/c1-5(7)3-2-4-6/h2-4H2,1H3 | C5H9O2 |
| C2H5COC2H4O | CCC(C(C)[O])=O  | InChI=1S/C5H9O2/c1-3-5(7)4(2)6/h4H,3H2,1-2H3 |  | C5H9O2 |
| CH3COCH2C2H4O | CC(CC(C)=O)[O]  | InChI=1S/C5H9O2/c1-4(6)3-5(2)7/h4H,3H2,1-2H3 |  | C5H9O2 |
| CHOCH2C3H6O | CCC(CC=O)[O]  | InChI=1S/C5H9O2/c1-2-5(7)3-4-6/h4-5H,2-3H2,1H3 |  | C5H9O2 |
| C2H5COCH2CH2O | CCC(CC[O])=O  | InChI=1S/C5H9O2/c1-2-5(7)3-4-6/h2-4H2,1H3 |  | C5H9O2 |
| C5H10OH-1 | CCC[CH]CO  | InChI=1S/C5H11O/c1-2-3-4-5-6/h4,6H,2-3,5H2,1H3 |  | C5H11O |
| C5H10OH-2 | CC[CH]C(C)O  | InChI=1S/C5H11O/c1-3-4-5(2)6/h4-6H,3H2,1-2H3 |  | C5H11O |
| O2C5H10OH-1 | CCCC(CO)O[O]  | InChI=1S/C5H11O3/c1-2-3-5(4-6)8-7/h5-6H,2-4H2,1H3 |  | C5H11O3 |
| O2C5H10OH-2 | CCC(C(C)O)O[O]  | InChI=1S/C5H11O3/c1-3-5(8-7)4(2)6/h4-6H,3H2,1-2H3 |  | C5H11O3 |
| IC5H12 | CCC(C)C  | InChI=1S/C5H12/c1-4-5(2)3/h5H,4H2,1-3H3 |  | C5H12 |
| AC5H11 | CCC([CH2])C  | InChI=1S/C5H11/c1-4-5(2)3/h5H,2,4H2,1,3H3 |  | C5H11 |
| BC5H11 | CC[C](C)C  | InChI=1S/C5H11/c1-4-5(2)3/h4H2,1-3H3 |  | C5H11 |
| CC5H11 | C[CH]C(C)C  | InChI=1S/C5H11/c1-4-5(2)3/h4-5H,1-3H3 |  | C5H11 |
| DC5H11 | [CH2]CC(C)C  | InChI=1S/C5H11/c1-4-5(2)3/h5H,1,4H2,2-3H3 |  | C5H11 |
| BC5H10 | CC=C(C)C  | InChI=1S/C5H10/c1-4-5(2)3/h4H,1-3H3 |  | C5H10 |
| CC5H10 | C=CC(C)C  | InChI=1S/C5H10/c1-4-5(2)3/h4-5H,1H2,2-3H3 |  | C5H10 |
| AC5H9O-A2 | CCC(=C)C[O]  | InChI=1S/C5H9O/c1-3-5(2)4-6/h2-4H2,1H3 |  | C5H9O |
| AC5H11O2H | CCC(C)COO  | InChI=1S/C5H12O2/c1-3-5(2)4-7-6/h5-6H,3-4H2,1-2H3 |  | C5H12O2 |
| BC5H11O2H | CCC(C)(C)OO  | InChI=1S/C5H12O2/c1-4-5(2,3)7-6/h6H,4H2,1-3H3 |  | C5H12O2 |
| CC5H11O2H | CC(C)C(C)OO  | InChI=1S/C5H12O2/c1-4(2)5(3)7-6/h4-6H,1-3H3 |  | C5H12O2 |
| DC5H11O2H | CC(C)CCOO  | InChI=1S/C5H12O2/c1-5(2)3-4-7-6/h5-6H,3-4H2,1-2H3 |  | C5H12O2 |
| AC5H11O2 | CCC(C)CO[O]  | InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h5H,3-4H2,1-2H3 |  | C5H11O2 |
| BC5H11O2 | CCC(C)(C)O[O]  | InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h4H2,1-3H3 |  | C5H11O2 |
| CC5H11O2 | CC(C)C(C)O[O]  | InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-5H,1-3H3 |  | C5H11O2 |
| DC5H11O2 | CC(C)CCO[O]  | InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h5H,3-4H2,1-2H3 |  | C5H11O2 |
| AC5H11O | CCC(C)C[O]  | InChI=1S/C5H11O/c1-3-5(2)4-6/h5H,3-4H2,1-2H3 |  | C5H11O |
| BC5H11O | CCC(C)(C)[O]  | InChI=1S/C5H11O/c1-4-5(2,3)6/h4H2,1-3H3 |  | C5H11O |
| CC5H11O | CC(C)C(C)[O]  | InChI=1S/C5H11O/c1-4(2)5(3)6/h4-5H,1-3H3 |  | C5H11O |
| DC5H11O | CC(C)CC[O]  | InChI=1S/C5H11O/c1-5(2)3-4-6/h5H,3-4H2,1-2H3 |  | C5H11O |
| AC5H10OOH-A | CCC([CH2])COO  | InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h5-6H,2-4H2,1H3 |  | C5H11O2 |
| AC5H10OOH-B | CC[C](C)COO  | InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h6H,3-4H2,1-2H3 |  | C5H11O2 |
| AC5H10OOH-C | C[CH]C(C)COO  | InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h3,5-6H,4H2,1-2H3 |  | C5H11O2 |
| AC5H10OOH-D | [CH2]CC(C)COO  | InChI=1S/C5H11O2/c1-3-5(2)4-7-6/h5-6H,1,3-4H2,2H3 |  | C5H11O2 |
| BC5H10OOH-A | CCC([CH2])(C)OO  | InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h6H,2,4H2,1,3H3 |  | C5H11O2 |
| BC5H10OOH-C | C[CH]C(C)(C)OO  | InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h4,6H,1-3H3 |  | C5H11O2 |
| BC5H10OOH-D | [CH2]CC(C)(C)OO  | InChI=1S/C5H11O2/c1-4-5(2,3)7-6/h6H,1,4H2,2-3H3 |  | C5H11O2 |
| CC5H10OOH-A | [CH2]C(C)C(C)OO  | InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-6H,1H2,2-3H3 |  | C5H11O2 |
| CC5H10OOH-B | C[C](C)C(C)OO  | InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h5-6H,1-3H3 |  | C5H11O2 |
| CC5H10OOH-D | CC(C)C([CH2])OO  | InChI=1S/C5H11O2/c1-4(2)5(3)7-6/h4-6H,3H2,1-2H3 |  | C5H11O2 |
| DC5H10OOH-A | [CH2]C(C)CCOO  | InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h5-6H,1,3-4H2,2H3 |  | C5H11O2 |
| DC5H10OOH-B | C[C](C)CCOO  | InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h6H,3-4H2,1-2H3 |  | C5H11O2 |
| DC5H10OOH-C | CC(C)[CH]COO  | InChI=1S/C5H11O2/c1-5(2)3-4-7-6/h3,5-6H,4H2,1-2H3 |  | C5H11O2 |
| A-AC5H10O | CCC1COC1  | InChI=1S/C5H10O/c1-2-5-3-6-4-5/h5H,2-4H2,1H3 |  | C5H10O |
| A-BC5H10O | CCC1(C)CO1  | InChI=1S/C5H10O/c1-3-5(2)4-6-5/h3-4H2,1-2H3 |  | C5H10O |
| A-CC5H10O | CC1COC1C  | InChI=1S/C5H10O/c1-4-3-6-5(4)2/h4-5H,3H2,1-2H3 |  | C5H10O |
| A-DC5H10O | CC1CCOC1  | InChI=1S/C5H10O/c1-5-2-3-6-4-5/h5H,2-4H2,1H3 |  | C5H10O |
| B-CC5H10O | CC1C(C)(C)O1  | InChI=1S/C5H10O/c1-4-5(2,3)6-4/h4H,1-3H3 |  | C5H10O |
| B-DC5H10O | CC1(C)CCO1  | InChI=1S/C5H10O/c1-5(2)3-4-6-5/h3-4H2,1-2H3 |  | C5H10O |
| C-DC5H10O | CC(C)C1CO1  | InChI=1S/C5H10O/c1-4(2)5-3-6-5/h4-5H,3H2,1-2H3 |  | C5H10O |
| AC5H10OOH-AO2 | CCC(COO)CO[O]  | InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h5-6H,2-4H2,1H3 |  | C5H11O4 |
| AC5H10OOH-BO2 | CCC(C)(COO)O[O]  | InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h6H,3-4H2,1-2H3 |  | C5H11O4 |
| AC5H10OOH-CO2 | CC(COO)C(C)O[O]  | InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-6H,3H2,1-2H3 |  | C5H11O4 |
| AC5H10OOH-DO2 | CC(CCO[O])COO  | InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h5,7H,2-4H2,1H3 |  | C5H11O4 |
| BC5H10OOH-AO2 | CCC(C)(CO[O])OO  | InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h7H,3-4H2,1-2H3 |  | C5H11O4 |
| BC5H10OOH-CO2 | CC(C(C)(C)OO)O[O]  | InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,7H,1-3H3 |  | C5H11O4 |
| BC5H10OOH-DO2 | CC(C)(CCO[O])OO  | InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h7H,3-4H2,1-2H3 |  | C5H11O4 |
| CC5H10OOH-AO2 | CC(CO[O])C(C)OO  | InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-5,7H,3H2,1-2H3 |  | C5H11O4 |
| CC5H10OOH-BO2 | CC(C(C)(C)O[O])OO  | InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,6H,1-3H3 |  | C5H11O4 |
| CC5H10OOH-DO2 | CC(C)C(CO[O])OO  | InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h4-5,7H,3H2,1-2H3 |  | C5H11O4 |
| DC5H10OOH-AO2 | CC(CCOO)CO[O]  | InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h5-6H,2-4H2,1H3 |  | C5H11O4 |
| DC5H10OOH-BO2 | CC(C)(CCOO)O[O]  | InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h6H,3-4H2,1-2H3 |  | C5H11O4 |
| DC5H10OOH-CO2 | CC(C)C(COO)O[O]  | InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h4-6H,3H2,1-2H3 |  | C5H11O4 |
| C5H9A-A,BOOH | CCC([CH2])(COO)OO  | InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h6-7H,2-4H2,1H3 |  | C5H11O4 |
| C5H9A-A,COOH | [CH2]C(COO)C(C)OO  | InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-7H,1,3H2,2H3 |  | C5H11O4 |
| C5H9A-A,DOOH | [CH2]C(CCOO)COO  | InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h5-7H,1-4H2 |  | C5H11O4 |
| C5H9A-B,COOH | CC(C([CH2])(C)OO)OO  | InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,6-7H,2H2,1,3H3 |  | C5H11O4 |
| C5H9A-B,DOOH | [CH2]C(C)(CCOO)OO  | InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h6-7H,1,3-4H2,2H3 |  | C5H11O4 |
| C5H9A-C,DOOH | [CH2]C(C)C(COO)OO  | InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h4-7H,1,3H2,2H3 |  | C5H11O4 |
| C5H9B-A,AOOH | CC[C](COO)COO  | InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h6-7H,2-4H2,1H3 |  | C5H11O4 |
| C5H9B-A,COOH | C[C](COO)C(C)OO  | InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h5-7H,3H2,1-2H3 |  | C5H11O4 |
| C5H9B-A,DOOH | C[C](CCOO)COO  | InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h6-7H,2-4H2,1H3 |  | C5H11O4 |
| C5H9B-C,DOOH | C[C](C)C(COO)OO  | InChI=1S/C5H11O4/c1-4(2)5(9-7)3-8-6/h5-7H,3H2,1-2H3 |  | C5H11O4 |
| C5H9C-A,AOOH | C[CH]C(COO)COO  | InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h2,5-7H,3-4H2,1H3 |  | C5H11O4 |
| C5H9C-A,BOOH | C[CH]C(C)(COO)OO  | InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h3,6-7H,4H2,1-2H3 |  | C5H11O4 |
| C5H9C-A,DOOH | CC([CH]COO)COO  | InChI=1S/C5H11O4/c1-5(4-9-7)2-3-8-6/h2,5-7H,3-4H2,1H3 |  | C5H11O4 |
| C5H9C-B,DOOH | CC(C)([CH]COO)OO  | InChI=1S/C5H11O4/c1-5(2,9-7)3-4-8-6/h3,6-7H,4H2,1-2H3 |  | C5H11O4 |
| C5H9D-A,AOOH | [CH2]CC(COO)COO  | InChI=1S/C5H11O4/c1-2-5(3-8-6)4-9-7/h5-7H,1-4H2 |  | C5H11O4 |
| C5H9D-A,BOOH | [CH2]CC(C)(COO)OO  | InChI=1S/C5H11O4/c1-3-5(2,9-7)4-8-6/h6-7H,1,3-4H2,2H3 |  | C5H11O4 |
| C5H9D-A,COOH | CC(COO)C([CH2])OO  | InChI=1S/C5H11O4/c1-4(3-8-6)5(2)9-7/h4-7H,2-3H2,1H3 |  | C5H11O4 |
| C5H9D-B,COOH | [CH2]C(C(C)(C)OO)OO  | InChI=1S/C5H11O4/c1-4(8-6)5(2,3)9-7/h4,6-7H,1H2,2-3H3 |  | C5H11O4 |
| C5H9A-AOOH | CCC(=C)COO  | InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h6H,2-4H2,1H3 |  | C5H10O2 |
| C5H9A-COOH | C=C(C)C(C)OO  | InChI=1S/C5H10O2/c1-4(2)5(3)7-6/h5-6H,1H2,2-3H3 |  | C5H10O2 |
| C5H9A-DOOH | C=C(C)CCOO  | InChI=1S/C5H10O2/c1-5(2)3-4-7-6/h6H,1,3-4H2,2H3 |  | C5H10O2 |
| C5H9B-AOOH | CC=C(C)COO  | InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h3,6H,4H2,1-2H3 |  | C5H10O2 |
| C5H9B-DOOH | CC(C)=CCOO  | InChI=1S/C5H10O2/c1-5(2)3-4-7-6/h3,6H,4H2,1-2H3 |  | C5H10O2 |
| C5H9C-AOOH | C=CC(C)COO  | InChI=1S/C5H10O2/c1-3-5(2)4-7-6/h3,5-6H,1,4H2,2H3 |  | C5H10O2 |
| C5H9C-BOOH | C=CC(C)(C)OO  | InChI=1S/C5H10O2/c1-4-5(2,3)7-6/h4,6H,1H2,2-3H3 |  | C5H10O2 |
| C5H9OA-AOOH-B | CCC1(COC1)OO  | InChI=1S/C5H10O3/c1-2-5(8-6)3-7-4-5/h6H,2-4H2,1H3 |  | C5H10O3 |
| C5H9OA-AOOH-C | CC(C1COC1)OO  | InChI=1S/C5H10O3/c1-4(8-6)5-2-7-3-5/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9OA-AOOH-D | C(COO)C1COC1  | InChI=1S/C5H10O3/c6-8-2-1-5-3-7-4-5/h5-6H,1-4H2 |  | C5H10O3 |
| C5H9OA-BOOH-A | CCC1(CO1)COO  | InChI=1S/C5H10O3/c1-2-5(3-7-5)4-8-6/h6H,2-4H2,1H3 |  | C5H10O3 |
| C5H9OA-BOOH-C | CC(C1(C)CO1)OO  | InChI=1S/C5H10O3/c1-4(8-6)5(2)3-7-5/h4,6H,3H2,1-2H3 |  | C5H10O3 |
| C5H9OA-BOOH-D | CC1(CCOO)CO1  | InChI=1S/C5H10O3/c1-5(4-7-5)2-3-8-6/h6H,2-4H2,1H3 |  | C5H10O3 |
| C5H9OA-COOH-A | CC1C(CO1)COO  | InChI=1S/C5H10O3/c1-4-5(2-7-4)3-8-6/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9OA-COOH-B | CC1C(C)(CO1)OO  | InChI=1S/C5H10O3/c1-4-5(2,8-6)3-7-4/h4,6H,3H2,1-2H3 |  | C5H10O3 |
| C5H9OA-COOH-D | CC1COC1COO  | InChI=1S/C5H10O3/c1-4-2-7-5(4)3-8-6/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9OA-DOOH-A | C1COCC1COO  | InChI=1S/C5H10O3/c6-8-4-5-1-2-7-3-5/h5-6H,1-4H2 |  | C5H10O3 |
| C5H9OA-DOOH-B | CC1(CCOC1)OO  | InChI=1S/C5H10O3/c1-5(8-6)2-3-7-4-5/h6H,2-4H2,1H3 | C5H10O3 |
| C5H9OA-DOOH-C | CC1COCC1OO  | InChI=1S/C5H10O3/c1-4-2-7-3-5(4)8-6/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9OB-COOH-A | CC1C(C)(COO)O1  | InChI=1S/C5H10O3/c1-4-5(2,8-4)3-7-6/h4,6H,3H2,1-2H3 |  | C5H10O3 |
| C5H9OB-COOH-D | CC1(C)C(COO)O1  | InChI=1S/C5H10O3/c1-5(2)4(8-5)3-7-6/h4,6H,3H2,1-2H3 |  | C5H10O3 |
| C5H9OB-DOOH-A | CC1(CCO1)COO  | InChI=1S/C5H10O3/c1-5(4-8-6)2-3-7-5/h6H,2-4H2,1H3 |  | C5H10O3 |
| C5H9OB-DOOH-C | CC1(C)C(CO1)OO  | InChI=1S/C5H10O3/c1-5(2)4(8-6)3-7-5/h4,6H,3H2,1-2H3 |  | C5H10O3 |
| C5H9OC-DOOH-A | CC(COO)C1CO1  | InChI=1S/C5H10O3/c1-4(2-8-6)5-3-7-5/h4-6H,2-3H2,1H3 |  | C5H10O3 |
| C5H9OC-DOOH-B | CC(C)(C1CO1)OO  | InChI=1S/C5H10O3/c1-5(2,8-6)4-3-7-4/h4,6H,3H2,1-2H3 |  | C5H10O3 |
| AC3H5OCH2 | C=CCO[CH2]  | InChI=1S/C4H7O/c1-3-4-5-2/h3H,1-2,4H2 |  | C4H7O |
| CH3COCH2OCH2CH2 | [CH2]COCC(C)=O  | InChI=1S/C5H9O2/c1-3-7-4-5(2)6/h1,3-4H2,2H3 |  | C5H9O2 |
| IC5KETAA | CCC(C=O)COO  | InChI=1S/C5H10O3/c1-2-5(3-6)4-8-7/h3,5,7H,2,4H2,1H3 |  | C5H10O3 |
| IC5KETAB | CCC(C)(C=O)OO  | InChI=1S/C5H10O3/c1-3-5(2,4-6)8-7/h4,7H,3H2,1-2H3 |  | C5H10O3 |
| IC5KETAC | CC(C=O)C(C)OO  | InChI=1S/C5H10O3/c1-4(3-6)5(2)8-7/h3-5,7H,1-2H3 |  | C5H10O3 |
| IC5KETAD | CC(CCOO)C=O  | InChI=1S/C5H10O3/c1-5(4-6)2-3-8-7/h4-5,7H,2-3H2,1H3 |  | C5H10O3 |
| IC5KETCA | CC(COO)C(C)=O  | InChI=1S/C5H10O3/c1-4(3-8-7)5(2)6/h4,7H,3H2,1-2H3 |  | C5H10O3 |
| IC5KETCB | CC(C(C)(C)OO)=O  | InChI=1S/C5H10O3/c1-4(6)5(2,3)8-7/h7H,1-3H3 |  | C5H10O3 |
| IC5KETCD | CC(C)C(COO)=O  | InChI=1S/C5H10O3/c1-4(2)5(6)3-8-7/h4,7H,3H2,1-2H3 |  | C5H10O3 |
| IC5KETDA | CC(CC=O)COO  | InChI=1S/C5H10O3/c1-5(2-3-6)4-8-7/h3,5,7H,2,4H2,1H3 |  | C5H10O3 |
| IC5KETDB | CC(C)(CC=O)OO  | InChI=1S/C5H10O3/c1-5(2,8-7)3-4-6/h4,7H,3H2,1-2H3 |  | C5H10O3 |
| IC5KETDC | CC(C)C(C=O)OO  | InChI=1S/C5H10O3/c1-4(2)5(3-6)8-7/h3-5,7H,1-2H3 |  | C5H10O3 |
| C2H5CH(CH2O)CHO | CCC(C=O)C[O]  | InChI=1S/C5H9O2/c1-2-5(3-6)4-7/h3,5H,2,4H2,1H3 |  | C5H9O2 |
| C3H5O(CH3)CHO | CCC(C)(C=O)[O]  | InChI=1S/C5H9O2/c1-3-5(2,7)4-6/h4H,3H2,1-2H3 |  | C5H9O2 |
| C2H4OCH(CH3)CHO | CC(C=O)C(C)[O]  | InChI=1S/C5H9O2/c1-4(3-6)5(2)7/h3-5H,1-2H3 |  | C5H9O2 |
| CH2OC3H6CHO | CC(CC[O])C=O  | InChI=1S/C5H9O2/c1-5(4-7)2-3-6/h4-5H,2-3H2,1H3 |  | C5H9O2 |
| CH3COCH(CH3)CH2O | CC(C[O])C(C)=O  | InChI=1S/C5H9O2/c1-4(3-6)5(2)7/h4H,3H2,1-2H3 |  | C5H9O2 |
| CH3CO(CH3)C2H3O | CC(C(C)(C)[O])=O  | InChI=1S/C5H9O2/c1-4(6)5(2,3)7/h1-3H3 |  | C5H9O2 |
| CH2OCOCH(CH3)CH3 | CC(C)C(C[O])=O  | InChI=1S/C5H9O2/c1-4(2)5(7)3-6/h4H,3H2,1-2H3 |  | C5H9O2 |
| CHOC3H6CH2O | CC(CC=O)C[O]  | InChI=1S/C5H9O2/c1-5(4-7)2-3-6/h3,5H,2,4H2,1H3 |  | C5H9O2 |
| CHOCH2(CH3)C2H3O | CC(C)(CC=O)[O]  | InChI=1S/C5H9O2/c1-5(2,7)3-4-6/h4H,3H2,1-2H3 |  | C5H9O2 |
| CHOCHOCH(CH3)CH3 | CC(C)C(C=O)[O]  | InChI=1S/C5H9O2/c1-4(2)5(7)3-6/h3-5H,1-2H3 |  | C5H9O2 |
| AC5H10OH | CC[C](C)CO  | InChI=1S/C5H11O/c1-3-5(2)4-6/h6H,3-4H2,1-2H3 |  | C5H11O |
| BC5H10OH | C[CH]C(C)(C)O  | InChI=1S/C5H11O/c1-4-5(2,3)6/h4,6H,1-3H3 |  | C5H11O |
| CC5H10OH | CC(C)C([CH2])O  | InChI=1S/C5H11O/c1-4(2)5(3)6/h4-6H,3H2,1-2H3 |  | C5H11O |
| AO2C5H10OH | CCC(C)(CO)O[O]  | InChI=1S/C5H11O3/c1-3-5(2,4-6)8-7/h6H,3-4H2,1-2H3 |  | C5H11O3 |
| BO2C5H10OH | CC(C(C)(C)O)O[O]  | InChI=1S/C5H11O3/c1-4(8-7)5(2,3)6/h4,6H,1-3H3 |  | C5H11O3 |
| CO2C5H10OH | CC(C)C(CO[O])O  | InChI=1S/C5H11O3/c1-4(2)5(6)3-8-7/h4-6H,3H2,1-2H3 |  | C5H11O3 |
| IC3H5COCH3 | C=C(C)C(C)=O  | InChI=1S/C5H8O/c1-4(2)5(3)6/h1H2,2-3H3 |  | C5H8O |
| IC3H5COCH2 | C=C(C)C(=C)[O]  | InChI=1S/C5H7O/c1-4(2)5(3)6/h1,3H2,2H3 |  | C5H7O |
| AC3H4COCH3 | C=C([CH2])C(C)=O  | InChI=1S/C5H7O/c1-4(2)5(3)6/h1-2H2,3H3 |  | C5H7O |
| NEOC5H12 | CC(C)(C)C  | InChI=1S/C5H12/c1-5(2,3)4/h1-4H3 |  | C5H12 |
| NEOC5H11 | [CH2]C(C)(C)C  | InChI=1S/C5H11/c1-5(2,3)4/h1H2,2-4H3 |  | C5H11 |
| NEOC5H11O2H | CC(C)(C)COO  | InChI=1S/C5H12O2/c1-5(2,3)4-7-6/h6H,4H2,1-3H3 |  | C5H12O2 |
| NEOC5H11O2 | CC(C)(C)CO[O]  | InChI=1S/C5H11O2/c1-5(2,3)4-7-6/h4H2,1-3H3 |  | C5H11O2 |
| NEOC5H11O | CC(C)(C)C[O]  | InChI=1S/C5H11O/c1-5(2,3)4-6/h4H2,1-3H3 |  | C5H11O |
| NEOC5H10OOH | [CH2]C(C)(C)COO  | InChI=1S/C5H11O2/c1-5(2,3)4-7-6/h6H,1,4H2,2-3H3 |  | C5H11O2 |
| NEO-C5H10O | CC1(C)COC1  | InChI=1S/C5H10O/c1-5(2)3-6-4-5/h3-4H2,1-2H3 |  | C5H10O |
| NEOC5H10OOH-O2 | CC(C)(COO)CO[O]  | InChI=1S/C5H11O4/c1-5(2,3-8-6)4-9-7/h6H,3-4H2,1-2H3 |  | C5H11O4 |
| NEOC5H9Q2 | [CH2]C(C)(COO)COO  | InChI=1S/C5H11O4/c1-5(2,3-8-6)4-9-7/h6-7H,1,3-4H2,2H3 |  | C5H11O4 |
| NEOC5KET | CC(C)(C=O)COO  | InChI=1S/C5H10O3/c1-5(2,3-6)4-8-7/h3,7H,4H2,1-2H3 |  | C5H10O3 |
| NEOC5KETOX | CC(C)(C=O)C[O]  | InChI=1S/C5H9O2/c1-5(2,3-6)4-7/h3H,4H2,1-2H3 |  | C5H9O2 |
| NEOC5KEJOL | CC(C)(CO)[C]=O  | InChI=1S/C5H9O2/c1-5(2,3-6)4-7/h6H,3H2,1-2H3 |  | C5H9O2 |
| NEOC5H9O-OOH | CC1(COC1)COO  | InChI=1S/C5H10O3/c1-5(4-8-6)2-7-3-5/h6H,2-4H2,1H3 |  | C5H10O3 |
| SC3H5OOH | C=C(C)OO  | InChI=1S/C3H6O2/c1-3(2)5-4/h4H,1H2,2H3 |  | C3H6O2 |
| C5H10OOH1-2O | C(OO)C([O])CCC | InChI=1S/C5H11O3/c1-2-3-5(6)4-8-7/h5,7H,2-4H2,1H3 |  | C5H11O3 |
| C5H10OOH1-3O | C(OO)CC([O])CC | InChI=1S/C5H11O3/c1-2-5(6)3-4-8-7/h5,7H,2-4H2,1H3 |  | C5H11O3 |
| C5H10OOH1-4O | C(OO)CCC([O])C | InChI=1S/C5H11O3/c1-5(6)3-2-4-8-7/h5,7H,2-4H2,1H3 |  | C5H11O3 |
| C5H10OOH1-5O | C(OO)CCCC([O]) | InChI=1S/C5H11O3/c6-4-2-1-3-5-8-7/h7H,1-5H2 |  | C5H11O3 |
| C5H10OOH2-1O | C([O])C(OO)CCC | InChI=1S/C5H11O3/c1-2-3-5(4-6)8-7/h5,7H,2-4H2,1H3 |  | C5H11O3 |
| C5H10OOH2-3O | CC(OO)C([O])CC | InChI=1S/C5H11O3/c1-3-5(6)4(2)8-7/h4-5,7H,3H2,1-2H3 |  | C5H11O3 |
| C5H10OOH2-4O | CC(OO)CC([O])C | InChI=1S/C5H11O3/c1-4(6)3-5(2)8-7/h4-5,7H,3H2,1-2H3 |  | C5H11O3 |
| C5H10OOH2-5O | CC(OO)CCC([O]) | InChI=1S/C5H11O3/c1-5(8-7)3-2-4-6/h5,7H,2-4H2,1H3 |  | C5H11O3 |
| C5H10OOH3-1O | CCC(OO)CC([O]) | InChI=1S/C5H11O3/c1-2-5(8-7)3-4-6/h5,7H,2-4H2,1H3 |  | C5H11O3 |
| C5H10OOH3-2O | CCC(OO)C([O])C | InChI=1S/C5H11O3/c1-3-5(8-7)4(2)6/h4-5,7H,3H2,1-2H3 |  | C5H11O3 |
| NC6H14 | CCCCCC | InChI=1S/C6H14/c1-3-5-6-4-2/h3-6H2,1-2H3 |  | C6H14 |
| C6H13-1 | [CH2]CCCCC | InChI=1S/C6H13/c1-3-5-6-4-2/h1,3-6H2,2H3 |  | C6H13 |
| C6H13-2 | C[CH]CCCC | InChI=1S/C6H13/c1-3-5-6-4-2/h3H,4-6H2,1-2H3 |  | C6H13 |
| C6H13-3 | CC[CH]CCC | InChI=1S/C6H13/c1-3-5-6-4-2/h5H,3-4,6H2,1-2H3 |  | C6H13 |
| C6H12-1 | C=CCCCC | InChI=1S/C6H12/c1-3-5-6-4-2/h3H,1,4-6H2,2H3 |  | C6H12 |
| C6H12-2 | CC=CCCC | InChI=1S/C6H12/c1-3-5-6-4-2/h3,5H,4,6H2,1-2H3 |  | C6H12 |
| C6H12-3 | CCC=CCC | InChI=1S/C6H12/c1-3-5-6-4-2/h5-6H,3-4H2,1-2H3 |  | C6H12 |
| C6H111-3 | C=C[CH]CCC | InChI=1S/C6H11/c1-3-5-6-4-2/h3,5H,1,4,6H2,2H3 |  | C6H11 |
| C6H111-4 | C=CC[CH]CC | InChI=1S/C6H11/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3 |  | C6H11 |
| C6H111-5 | C=CCC[CH]C | InChI=1S/C6H11/c1-3-5-6-4-2/h3-4H,1,5-6H2,2H3 |  | C6H11 |
| C6H111-6 | C=CCCC[CH2] | InChI=1S/C6H11/c1-3-5-6-4-2/h3H,1-2,4-6H2 |  | C6H11 |
| C6H112-4 | CC=C[CH]CC | InChI=1S/C6H11/c1-3-5-6-4-2/h3,5-6H,4H2,1-2H3 |  | C6H11 |
| C6H112-5 | CC=CC[CH]C | InChI=1S/C6H11/c1-3-5-6-4-2/h3-5H,6H2,1-2H3 |  | C6H11 |
| C6H112-6 | CC=CCC[CH2] | InChI=1S/C6H11/c1-3-5-6-4-2/h4,6H,1,3,5H2,2H3 |  | C6H11 |
| C6H113-1 | CCC=CC[CH2] | InChI=1S/C6H11/c1-3-5-6-4-2/h5-6H,1,3-4H2,2H3 |  | C6H11 |
| C6H12OH-1J2 | C(O)[CH]CCCC | InChI=1S/C6H13O/c1-2-3-4-5-6-7/h5,7H,2-4,6H2,1H3 |  | C6H13O |
| C6H12OH-2J1 | [CH2]C(O)CCCC | InChI=1S/C6H13O/c1-3-4-5-6(2)7/h6-7H,2-5H2,1H3 |  | C6H13O |
| C6H12OH-2J3 | CC(O)[CH]CCC | InChI=1S/C6H13O/c1-3-4-5-6(2)7/h5-7H,3-4H2,1-2H3 |  | C6H13O |
| C6H12OH-3J2 | C[CH]C(O)CCC | InChI=1S/C6H13O/c1-3-5-6(7)4-2/h4,6-7H,3,5H2,1-2H3 |  | C6H13O |
| C6H12OH-3J4 | CCC(O)[CH]CC | InChI=1S/C6H13O/c1-3-5-6(7)4-2/h5-7H,3-4H2,1-2H3 |  | C6H13O |
| C6H12OH-1O2-2 | C(O)C(O[O])CCCC | InChI=1S/C6H13O3/c1-2-3-4-6(5-7)9-8/h6-7H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OH-2O2-1 | C(O[O])C(O)CCCC | InChI=1S/C6H13O3/c1-2-3-4-6(7)5-9-8/h6-7H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OH-2O2-3 | CC(O)C(O[O])CCC | InChI=1S/C6H13O3/c1-3-4-6(9-8)5(2)7/h5-7H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OH-3O2-2 | CC(O[O])C(O)CCC | InChI=1S/C6H13O3/c1-3-4-6(7)5(2)9-8/h5-7H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OH-3O2-4 | CCC(O)C(O[O])CC | InChI=1S/C6H13O3/c1-3-5(7)6(4-2)9-8/h5-7H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H11-1D3O | C=CC([O])CCC | InChI=1S/C6H11O/c1-3-5-6(7)4-2/h4,6H,2-3,5H2,1H3 |  | C6H11O |
| C6H11-1D4O | C=CCC([O])CC | InChI=1S/C6H11O/c1-3-5-6(7)4-2/h3,6H,1,4-5H2,2H3 |  | C6H11O |
| C6H11-1D5O | C=CCCC([O])C | InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3,6H,1,4-5H2,2H3 |  | C6H11O |
| C6H11-1D6O | C=CCCCC([O]) | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2H,1,3-6H2 |  | C6H11O |
| C6H11-2D1O | C([O])C=CCCC | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4-5H,2-3,6H2,1H3 |  | C6H11O |
| C6H11-2D4O | CC=CC([O])CC | InChI=1S/C6H11O/c1-3-5-6(7)4-2/h3,5-6H,4H2,1-2H3 |  | C6H11O |
| C6H11-2D5O | CC=CCC([O])C | InChI=1S/C6H11O/c1-3-4-5-6(2)7/h3-4,6H,5H2,1-2H3 |  | C6H11O |
| C6H11-2D6O | CC=CCCC([O]) | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-3H,4-6H2,1H3 |  | C6H11O |
| C6H11-3D1O | CCC=CCC([O]) | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3-4H,2,5-6H2,1H3 |  | C6H11O |
| C6H11-3D2O | CCC=CC([O])C | InChI=1S/C6H11O/c1-3-4-5-6(2)7/h4-6H,3H2,1-2H3 |  | C6H11O |
| C6H13OOH-1 | C(OO)CCCCC | InChI=1S/C6H14O2/c1-2-3-4-5-6-8-7/h7H,2-6H2,1H3 |  | C6H14O2 |
| C6H13OOH-2 | CC(OO)CCCC | InChI=1S/C6H14O2/c1-3-4-5-6(2)8-7/h6-7H,3-5H2,1-2H3 |  | C6H14O2 |
| C6H13OOH-3 | CCC(OO)CCC | InChI=1S/C6H14O2/c1-3-5-6(4-2)8-7/h6-7H,3-5H2,1-2H3 |  | C6H14O2 |
| C6H13O2-1 | C(O[O])CCCCC | InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h2-6H2,1H3 |  | C6H13O2 |
| C6H13O2-2 | CC(O[O])CCCC | InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6H,3-5H2,1-2H3 |  | C6H13O2 |
| C6H13O2-3 | CCC(O[O])CCC | InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6H,3-5H2,1-2H3 |  | C6H13O2 |
| C6H13O-1 | C([O])CCCCC | InChI=1S/C6H13O/c1-2-3-4-5-6-7/h2-6H2,1H3 |  | C6H13O |
| C6H13O-2 | CC([O])CCCC | InChI=1S/C6H13O/c1-3-4-5-6(2)7/h6H,3-5H2,1-2H3 |  | C6H13O |
| C6H13O-3 | CCC([O])CCC | InChI=1S/C6H13O/c1-3-5-6(7)4-2/h6H,3-5H2,1-2H3 |  | C6H13O |
| C6H12OOH1-2 | C(OO)[CH]CCCC | InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h5,7H,2-4,6H2,1H3 |  | C6H13O2 |
| C6H12OOH1-3 | C(OO)C[CH]CCC | InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h4,7H,2-3,5-6H2,1H3 |  | C6H13O2 |
| C6H12OOH1-4 | C(OO)CC[CH]CC | InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h3,7H,2,4-6H2,1H3 |  | C6H13O2 |
| C6H12OOH1-5 | C(OO)CCC[CH]C | InChI=1S/C6H13O2/c1-2-3-4-5-6-8-7/h2,7H,3-6H2,1H3 |  | C6H13O2 |
| C6H12OOH2-1 | [CH2]C(OO)CCCC | InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6-7H,2-5H2,1H3 |  | C6H13O2 |
| C6H12OOH2-3 | CC(OO)[CH]CCC | InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h5-7H,3-4H2,1-2H3 |  | C6H13O2 |
| C6H12OOH2-4 | CC(OO)C[CH]CC | InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h4,6-7H,3,5H2,1-2H3 |  | C6H13O2 |
| C6H12OOH2-5 | CC(OO)CC[CH]C | InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h3,6-7H,4-5H2,1-2H3 |  | C6H13O2 |
| C6H12OOH2-6 | CC(OO)CCC[CH2] | InChI=1S/C6H13O2/c1-3-4-5-6(2)8-7/h6-7H,1,3-5H2,2H3 |  | C6H13O2 |
| C6H12OOH3-1 | [CH2]CC(OO)CCC | InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6-7H,2-5H2,1H3 |  | C6H13O2 |
| C6H12OOH3-2 | C[CH]C(OO)CCC | InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h4,6-7H,3,5H2,1-2H3 |  | C6H13O2 |
| C6H12OOH3-4 | CCC(OO)[CH]CC | InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h5-7H,3-4H2,1-2H3 |  | C6H13O2 |
| C6H12OOH3-5 | CCC(OO)C[CH]C | InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h3,6-7H,4-5H2,1-2H3 |  | C6H13O2 |
| C6H12OOH3-6 | CCC(OO)CC[CH2] | InChI=1S/C6H13O2/c1-3-5-6(4-2)8-7/h6-7H,1,3-5H2,2H3 |  | C6H13O2 |
| C6H12O1-2 | C1C(O1)CCCC | InChI=1S/C6H12O/c1-2-3-4-6-5-7-6/h6H,2-5H2,1H3 |  | C6H12O |
| C6H12O1-3 | C1CC(O1)CCC | InChI=1S/C6H12O/c1-2-3-6-4-5-7-6/h6H,2-5H2,1H3 |  | C6H12O |
| C6H12O1-4 | C1CCC(O1)CC | InChI=1S/C6H12O/c1-2-6-4-3-5-7-6/h6H,2-5H2,1H3 |  | C6H12O |
| C6H12O1-5 | C1CCCC(O1)C | InChI=1S/C6H12O/c1-6-4-2-3-5-7-6/h6H,2-5H2,1H3 |  | C6H12O |
| C6H12O2-3 | CC1C(O1)CCC | InChI=1S/C6H12O/c1-3-4-6-5(2)7-6/h5-6H,3-4H2,1-2H3 |  | C6H12O |
| C6H12O2-4 | CC1CC(O1)CC | InChI=1S/C6H12O/c1-3-6-4-5(2)7-6/h5-6H,3-4H2,1-2H3 |  | C6H12O |
| C6H12O2-5 | CC1CCC(O1)C | InChI=1S/C6H12O/c1-5-3-4-6(2)7-5/h5-6H,3-4H2,1-2H3 |  | C6H12O |
| C6H12O3-4 | CCC1C(O1)CC | InChI=1S/C6H12O/c1-3-5-6(4-2)7-5/h5-6H,3-4H2,1-2H3 |  | C6H12O |
| C6H12OOH1-2O2 | C(OO)C(O[O])CCCC | InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h6-7H,2-5H2,1H3 |  | C6H13O4 |
| C6H12OOH1-3O2 | C(OO)CC(O[O])CCC | InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6-7H,2-5H2,1H3 |  | C6H13O4 |
| C6H12OOH1-4O2 | C(OO)CCC(O[O])CC | InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6-7H,2-5H2,1H3 |  | C6H13O4 |
| C6H12OOH1-5O2 | C(OO)CCCC(O[O])C | InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6-7H,2-5H2,1H3 |  | C6H13O4 |
| C6H12OOH2-1O2 | C(O[O])C(OO)CCCC | InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h6,8H,2-5H2,1H3 |  | C6H13O4 |
| C6H12OOH2-3O2 | CC(OO)C(O[O])CCC | InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-7H,3-4H2,1-2H3 |  | C6H13O4 |
| C6H12OOH2-4O2 | CC(OO)CC(O[O])CC | InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-7H,3-4H2,1-2H3 |  | C6H13O4 |
| C6H12OOH2-5O2 | CC(OO)CCC(O[O])C | InChI=1S/C6H13O4/c1-5(9-7)3-4-6(2)10-8/h5-7H,3-4H2,1-2H3 |  | C6H13O4 |
| C6H12OOH2-6O2 | CC(OO)CCCC(O[O]) | InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6,8H,2-5H2,1H3 |  | C6H13O4 |
| C6H12OOH3-1O2 | C(O[O])CC(OO)CCC | InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6,8H,2-5H2,1H3 |  | C6H13O4 |
| C6H12OOH3-2O2 | CC(O[O])C(OO)CCC | InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-6,8H,3-4H2,1-2H3 |  | C6H13O4 |
| C6H12OOH3-4O2 | CCC(OO)C(O[O])CC | InChI=1S/C6H13O4/c1-3-5(9-7)6(4-2)10-8/h5-7H,3-4H2,1-2H3 |  | C6H13O4 |
| C6H12OOH3-5O2 | CCC(OO)CC(O[O])C | InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-6,8H,3-4H2,1-2H3 |  | C6H13O4 |
| C6H12OOH3-6O2 | CCC(OO)CCC(O[O]) | InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6,8H,2-5H2,1H3 |  | C6H13O4 |
| C6H11-1D3OOH | C=CC(OO)CCC | InChI=1S/C6H12O2/c1-3-5-6(4-2)8-7/h4,6-7H,2-3,5H2,1H3 |  | C6H12O2 |
| C6H11-1D4OOH | C=CCC(OO)CC | InChI=1S/C6H12O2/c1-3-5-6(4-2)8-7/h3,6-7H,1,4-5H2,2H3 |  | C6H12O2 |
| C6H11-1D5OOH | C=CCCC(OO)C | InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h3,6-7H,1,4-5H2,2H3 |  | C6H12O2 |
| C6H11-1D6OOH | C=CCCCC(OO) | InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h2,7H,1,3-6H2 |  | C6H12O2 |
| C6H11-2D1OOH | C(OO)C=CCCC | InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h4-5,7H,2-3,6H2,1H3 |  | C6H12O2 |
| C6H11-2D4OOH | CC=CC(OO)CC | InChI=1S/C6H12O2/c1-3-5-6(4-2)8-7/h3,5-7H,4H2,1-2H3 |  | C6H12O2 |
| C6H11-2D5OOH | CC=CCC(OO)C | InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h3-4,6-7H,5H2,1-2H3 |  | C6H12O2 |
| C6H11-2D6OOH | CC=CCCC(OO) | InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h2-3,7H,4-6H2,1H3 |  | C6H12O2 |
| C6H11-3D1OOH | C(OO)CC=CCC | InChI=1S/C6H12O2/c1-2-3-4-5-6-8-7/h3-4,7H,2,5-6H2,1H3 |  | C6H12O2 |
| C6H11-3D2OOH | CC(OO)C=CCC | InChI=1S/C6H12O2/c1-3-4-5-6(2)8-7/h4-7H,3H2,1-2H3 |  | C6H12O2 |
| C6H11Q12-3 | C(OO)C(OO)[CH]CCC | InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h4,6-8H,2-3,5H2,1H3 |  | C6H13O4 |
| C6H11Q12-4 | C(OO)C(OO)C[CH]CC | InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h3,6-8H,2,4-5H2,1H3 |  | C6H13O4 |
| C6H11Q12-5 | C(OO)C(OO)CC[CH]C | InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h2,6-8H,3-5H2,1H3 |  | C6H13O4 |
| C6H11Q12-6 | C(OO)C(OO)CCC[CH2] | InChI=1S/C6H13O4/c1-2-3-4-6(10-8)5-9-7/h6-8H,1-5H2 |  | C6H13O4 |
| C6H11Q13-2 | C(OO)[CH]C(OO)CCC | InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h4,6-8H,2-3,5H2,1H3 |  | C6H13O4 |
| C6H11Q13-4 | C(OO)CC(OO)[CH]CC | InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h3,6-8H,2,4-5H2,1H3 |  | C6H13O4 |
| C6H11Q13-5 | C(OO)CC(OO)C[CH]C | InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h2,6-8H,3-5H2,1H3 |  | C6H13O4 |
| C6H11Q13-6 | C(OO)CC(OO)CC[CH2] | InChI=1S/C6H13O4/c1-2-3-6(10-8)4-5-9-7/h6-8H,1-5H2 |  | C6H13O4 |
| C6H11Q14-2 | C(OO)[CH]CC(OO)CC | InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h3,6-8H,2,4-5H2,1H3 |  | C6H13O4 |
| C6H11Q14-3 | C(OO)C[CH]C(OO)CC | InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h4,6-8H,2-3,5H2,1H3 |  | C6H13O4 |
| C6H11Q14-5 | C(OO)CCC(OO)[CH]C | InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h2,6-8H,3-5H2,1H3 |  | C6H13O4 |
| C6H11Q14-6 | C(OO)CCC(OO)C[CH2] | InChI=1S/C6H13O4/c1-2-6(10-8)4-3-5-9-7/h6-8H,1-5H2 |  | C6H13O4 |
| C6H11Q15-2 | C(OO)[CH]CCC(OO)C | InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h3,6-8H,2,4-5H2,1H3 |  | C6H13O4 |
| C6H11Q15-3 | C(OO)C[CH]CC(OO)C | InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h2,6-8H,3-5H2,1H3 |  | C6H13O4 |
| C6H11Q15-4 | C(OO)CC[CH]C(OO)C | InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h4,6-8H,2-3,5H2,1H3 |  | C6H13O4 |
| C6H11Q15-6 | C(OO)CCCC(OO)[CH2] | InChI=1S/C6H13O4/c1-6(10-8)4-2-3-5-9-7/h6-8H,1-5H2 |  | C6H13O4 |
| C6H11Q23-1 | [CH2]C(OO)C(OO)CCC | InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-8H,2-4H2,1H3 |  | C6H13O4 |
| C6H11Q23-4 | CC(OO)C(OO)[CH]CC | InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h4-8H,3H2,1-2H3 |  | C6H13O4 |
| C6H11Q23-5 | CC(OO)C(OO)C[CH]C | InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h3,5-8H,4H2,1-2H3 |  | C6H13O4 |
| C6H11Q23-6 | CC(OO)C(OO)CC[CH2] | InChI=1S/C6H13O4/c1-3-4-6(10-8)5(2)9-7/h5-8H,1,3-4H2,2H3 |  | C6H13O4 |
| C6H11Q24-1 | [CH2]C(OO)CC(OO)CC | InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-8H,2-4H2,1H3 |  | C6H13O4 |
| C6H11Q24-3 | CC(OO)[CH]C(OO)CC | InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h4-8H,3H2,1-2H3 |  | C6H13O4 |
| C6H11Q24-5 | CC(OO)CC(OO)[CH]C | InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h3,5-8H,4H2,1-2H3 |  | C6H13O4 |
| C6H11Q24-6 | CC(OO)CC(OO)C[CH2] | InChI=1S/C6H13O4/c1-3-6(10-8)4-5(2)9-7/h5-8H,1,3-4H2,2H3 |  | C6H13O4 |
| C6H11Q25-1 | [CH2]C(OO)CCC(OO)C | InChI=1S/C6H13O4/c1-5(9-7)3-4-6(2)10-8/h5-8H,1,3-4H2,2H3 |  | C6H13O4 |
| C6H11Q25-3 | CC(OO)[CH]CC(OO)C | InChI=1S/C6H13O4/c1-5(9-7)3-4-6(2)10-8/h3,5-8H,4H2,1-2H3 |  | C6H13O4 |
| C6H11Q34-1 | [CH2]CC(OO)C(OO)CC | InChI=1S/C6H13O4/c1-3-5(9-7)6(4-2)10-8/h5-8H,1,3-4H2,2H3 |  | C6H13O4 |
| C6H11Q34-2 | C[CH]C(OO)C(OO)CC | InChI=1S/C6H13O4/c1-3-5(9-7)6(4-2)10-8/h3,5-8H,4H2,1-2H3 |  | C6H13O4 |
| C6KET12 | C(=O)C(OO)CCCC | InChI=1S/C6H12O3/c1-2-3-4-6(5-7)9-8/h5-6,8H,2-4H2,1H3 |  | C6H12O3 |
| C6KET13 | C(=O)CC(OO)CCC | InChI=1S/C6H12O3/c1-2-3-6(9-8)4-5-7/h5-6,8H,2-4H2,1H3 | C6H12O3 |
| C6KET14 | C(=O)CCC(OO)CC | InChI=1S/C6H12O3/c1-2-6(9-8)4-3-5-7/h5-6,8H,2-4H2,1H3 |  | C6H12O3 |
| C6KET15 | C(=O)CCCC(OO)C | InChI=1S/C6H12O3/c1-6(9-8)4-2-3-5-7/h5-6,8H,2-4H2,1H3 |  | C6H12O3 |
| C6KET21 | C(OO)C(=O)CCCC | InChI=1S/C6H12O3/c1-2-3-4-6(7)5-9-8/h8H,2-5H2,1H3 |  | C6H12O3 |
| C6KET23 | CC(=O)C(OO)CCC | InChI=1S/C6H12O3/c1-3-4-6(9-8)5(2)7/h6,8H,3-4H2,1-2H3 |  | C6H12O3 |
| C6KET24 | CC(=O)CC(OO)CC | InChI=1S/C6H12O3/c1-3-6(9-8)4-5(2)7/h6,8H,3-4H2,1-2H3 |  | C6H12O3 |
| C6KET25 | CC(=O)CCC(OO)C | InChI=1S/C6H12O3/c1-5(7)3-4-6(2)9-8/h6,8H,3-4H2,1-2H3 |  | C6H12O3 |
| C6KET26 | CC(=O)CCCC(OO) | InChI=1S/C6H12O3/c1-6(7)4-2-3-5-9-8/h8H,2-5H2,1H3 |  | C6H12O3 |
| C6KET31 | C(OO)CC(=O)CCC | InChI=1S/C6H12O3/c1-2-3-6(7)4-5-9-8/h8H,2-5H2,1H3 |  | C6H12O3 |
| C6KET32 | CC(OO)C(=O)CCC | InChI=1S/C6H12O3/c1-3-4-6(7)5(2)9-8/h5,8H,3-4H2,1-2H3 |  | C6H12O3 |
| C6KET34 | CCC(=O)C(OO)CC | InChI=1S/C6H12O3/c1-3-5(7)6(4-2)9-8/h6,8H,3-4H2,1-2H3 |  | C6H12O3 |
| C6KET35 | CCC(=O)CC(OO)C | InChI=1S/C6H12O3/c1-3-6(7)4-5(2)9-8/h5,8H,3-4H2,1-2H3 |  | C6H12O3 |
| C6KET36 | CCC(=O)CCC(OO) | InChI=1S/C6H12O3/c1-2-6(7)4-3-5-9-8/h8H,2-5H2,1H3 |  | C6H12O3 |
| C5Y2 | CC(=O)CCC | InChI=1S/C5H10O/c1-3-4-5(2)6/h3-4H2,1-2H3 |  | C5H10O |
| C5Y2-1J | [CH2]C(=O)CCC | InChI=1S/C5H9O/c1-3-4-5(2)6/h2-4H2,1H3 |  | C5H9O |
| C5Y2-5J | CC(=O)CC[CH2] | InChI=1S/C5H9O/c1-3-4-5(2)6/h1,3-4H2,2H3 |  | C5H9O |
| C5Y3-1J | CCC(=O)C[CH2] | InChI=1S/C5H9O/c1-3-5(6)4-2/h1,3-4H2,2H3 |  | C5H9O |
| C5H91-1 | CCCC=[CH] | InChI=1S/C5H9/c1-3-5-4-2/h1,3H,4-5H2,2H3 |  | C5H9 |
| C5AL-4D | C(=O)CCC=C | InChI=1S/C5H8O/c1-2-3-4-5-6/h2,5H,1,3-4H2 |  | C5H8O |
| C5AL-2D | C(=O)CC=CC | InChI=1S/C5H8O/c1-2-3-4-5-6/h2-3,5H,4H2,1H3 |  | C5H8O |
| C6H11O12-3OOH | C1C(O1)C(OO)CCC | InChI=1S/C6H12O3/c1-2-3-5(9-7)6-4-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O12-4OOH | C1C(O1)CC(OO)CC | InChI=1S/C6H12O3/c1-2-5(9-7)3-6-4-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O12-5OOH | C1C(O1)CCC(OO)C | InChI=1S/C6H12O3/c1-5(9-7)2-3-6-4-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O12-6OOH | C1C(O1)CCCC(OO) | InChI=1S/C6H12O3/c7-9-4-2-1-3-6-5-8-6/h6-7H,1-5H2 |  | C6H12O3 |
| C6H11O13-2OOH | C1C(OO)C(O1)CCC | InChI=1S/C6H12O3/c1-2-3-5-6(9-7)4-8-5/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O13-4OOH | C1CC(O1)C(OO)CC | InChI=1S/C6H12O3/c1-2-5(9-7)6-3-4-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O13-5OOH | C1CC(O1)CC(OO)C | InChI=1S/C6H12O3/c1-5(9-7)4-6-2-3-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O13-6OOH | C1CC(O1)CCC(OO) | InChI=1S/C6H12O3/c7-9-4-1-2-6-3-5-8-6/h6-7H,1-5H2 |  | C6H12O3 |
| C6H11O14-2OOH | C1C(OO)CC(O1)CC | InChI=1S/C6H12O3/c1-2-5-3-6(9-7)4-8-5/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O14-3OOH | C1CC(OO)C(O1)CC | InChI=1S/C6H12O3/c1-2-5-6(9-7)3-4-8-5/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O14-5OOH | C1CCC(O1)C(OO)C | InChI=1S/C6H12O3/c1-5(9-7)6-3-2-4-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O14-6OOH | C1CCC(O1)CC(OO) | InChI=1S/C6H12O3/c7-9-5-3-6-2-1-4-8-6/h6-7H,1-5H2 |  | C6H12O3 |
| C6H11O15-2OOH | C1C(OO)CCC(O1)C | InChI=1S/C6H12O3/c1-5-2-3-6(9-7)4-8-5/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O15-3OOH | C1CC(OO)CC(O1)C | InChI=1S/C6H12O3/c1-5-4-6(9-7)2-3-8-5/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O15-4OOH | C1CCC(OO)C(O1)C | InChI=1S/C6H12O3/c1-5-6(9-7)3-2-4-8-5/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O15-6OOH | C1CCCC(O1)C(OO) | InChI=1S/C6H12O3/c7-9-5-6-3-1-2-4-8-6/h6-7H,1-5H2 |  | C6H12O3 |
| C6H11O23-1OOH | C(OO)C1C(O1)CCC | InChI=1S/C6H12O3/c1-2-3-5-6(9-5)4-8-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O23-4OOH | CC1C(O1)C(OO)CC | InChI=1S/C6H12O3/c1-3-5(9-7)6-4(2)8-6/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| C6H11O23-5OOH | CC1C(O1)CC(OO)C | InChI=1S/C6H12O3/c1-4(9-7)3-6-5(2)8-6/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| C6H11O23-6OOH | CC1C(O1)CCC(OO) | InChI=1S/C6H12O3/c1-5-6(9-5)3-2-4-8-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O24-1OOH | C(OO)C1CC(O1)CC | InChI=1S/C6H12O3/c1-2-5-3-6(9-5)4-8-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O24-3OOH | CC1C(OO)C(O1)CC | InChI=1S/C6H12O3/c1-3-5-6(9-7)4(2)8-5/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| C6H11O24-5OOH | CC1CC(O1)C(OO)C | InChI=1S/C6H12O3/c1-4-3-6(8-4)5(2)9-7/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| C6H11O24-6OOH | CC1CC(O1)CC(OO) | InChI=1S/C6H12O3/c1-5-4-6(9-5)2-3-8-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O25-1OOH | C(OO)C1CCC(O1)C | InChI=1S/C6H12O3/c1-5-2-3-6(9-5)4-8-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O25-3OOH | CC1C(OO)CC(O1)C | InChI=1S/C6H12O3/c1-4-3-6(9-7)5(2)8-4/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| C6H11O34-1OOH | C(OO)CC1C(O1)CC | InChI=1S/C6H12O3/c1-2-5-6(9-5)3-4-8-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| C6H11O34-2OOH | CC(OO)C1C(O1)CC | InChI=1S/C6H12O3/c1-3-5-6(8-5)4(2)9-7/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| PC4H9CHO | CCCCC=O | InChI=1S/C5H10O/c1-2-3-4-5-6/h5H,2-4H2,1H3 |  | C5H10O |
| PC4H8CHO-1 | CCC[CH]C=O | InChI=1S/C5H9O/c1-2-3-4-5-6/h4-5H,2-3H2,1H3 |  | C5H9O |
| PC4H8CHO-2 | CC[CH]CC=O | InChI=1S/C5H9O/c1-2-3-4-5-6/h3,5H,2,4H2,1H3 |  | C5H9O |
| PC4H8CHO-3 | C[CH]CCC=O | InChI=1S/C5H9O/c1-2-3-4-5-6/h2,5H,3-4H2,1H3 |  | C5H9O |
| PC4H8CHO-4 | [CH2]CCCC=O | InChI=1S/C5H9O/c1-2-3-4-5-6/h5H,1-4H2 |  | C5H9O |
| C4H7O12-4 | C1C(O1)C[CH2] | InChI=1S/C4H7O/c1-2-4-3-5-4/h4H,1-3H2 |  | C4H7O |
| C4H7O13-4 | C1CC(O1)[CH2] | InChI=1S/C4H7O/c1-4-2-3-5-4/h4H,1-3H2 |  | C4H7O |
| C4H7O23-1 | CC1C(O1)[CH2] | InChI=1S/C4H7O/c1-3-4(2)5-3/h3-4H,1H2,2H3 |  | C4H7O |
| C5H9O12-5 | C1C(O1)CC[CH2] | InChI=1S/C5H9O/c1-2-3-5-4-6-5/h5H,1-4H2 |  | C5H9O |
| C5H9O13-5 | C1CC(O1)C[CH2] | InChI=1S/C5H9O/c1-2-5-3-4-6-5/h5H,1-4H2 |  | C5H9O |
| C5H9O14-5 | C1CCC(O1)[CH2] | InChI=1S/C5H9O/c1-5-3-2-4-6-5/h5H,1-4H2 |  | C5H9O |
| C5H9O23-1 | CCC1C(O1)[CH2] | InChI=1S/C5H9O/c1-3-5-4(2)6-5/h4-5H,2-3H2,1H3 |  | C5H9O |
| C5H9O23-5 | [CH2]CC1C(O1)C | InChI=1S/C5H9O/c1-3-5-4(2)6-5/h4-5H,1,3H2,2H3 |  | C5H9O |
| C5H9O24-1 | [CH2]C1CC(O1)C | InChI=1S/C5H9O/c1-4-3-5(2)6-4/h4-5H,1,3H2,2H3 |  | C5H9O |
| C3H6CHO-3O | C([O])CCC=O | InChI=1S/C4H7O2/c5-3-1-2-4-6/h3H,1-2,4H2 |  | C4H7O2 |
| AC3H5CHO | C=CCC=O | InChI=1S/C4H6O/c1-2-3-4-5/h2,4H,1,3H2 |  | C4H6O |
| PC4H9CO | CCCC[C]=O | InChI=1S/C5H9O/c1-2-3-4-5-6/h2-4H2,1H3 |  | C5H9O |
| C6KET12O | C(=O)C([O])CCCC | InChI=1S/C6H11O2/c1-2-3-4-6(8)5-7/h5-6H,2-4H2,1H3 |  | C6H11O2 |
| C6KET13O | C(=O)CC([O])CCC | InChI=1S/C6H11O2/c1-2-3-6(8)4-5-7/h5-6H,2-4H2,1H3 | C6H11O2 |
| C6KET14O | C(=O)CCC([O])CC | InChI=1S/C6H11O2/c1-2-6(8)4-3-5-7/h5-6H,2-4H2,1H3 |  | C6H11O2 |
| C6KET15O | C(=O)CCCC([O])C | InChI=1S/C6H11O2/c1-6(8)4-2-3-5-7/h5-6H,2-4H2,1H3 | C6H11O2 |
| C6KET21O | C([O])C(=O)CCCC | InChI=1S/C6H11O2/c1-2-3-4-6(8)5-7/h2-5H2,1H3 |  | C6H11O2 |
| C6KET23O | CC(=O)C([O])CCC | InChI=1S/C6H11O2/c1-3-4-6(8)5(2)7/h6H,3-4H2,1-2H3 |  | C6H11O2 |
| C6KET24O | CC(=O)CC([O])CC | InChI=1S/C6H11O2/c1-3-6(8)4-5(2)7/h6H,3-4H2,1-2H3 | C6H11O2 |
| C6KET25O | CC(=O)CCC([O])C | InChI=1S/C6H11O2/c1-5(7)3-4-6(2)8/h5H,3-4H2,1-2H3 |  | C6H11O2 |
| C6KET26O | CC(=O)CCCC([O]) | InChI=1S/C6H11O2/c1-6(8)4-2-3-5-7/h2-5H2,1H3 |  | C6H11O2 |
| C6KET31O | CCCC(=O)CC([O]) | InChI=1S/C6H11O2/c1-2-3-6(8)4-5-7/h2-5H2,1H3 |  | C6H11O2 |
| C6KET32O | CCCC(=O)C([O])C | InChI=1S/C6H11O2/c1-3-4-6(8)5(2)7/h5H,3-4H2,1-2H3 |  | C6H11O2 |
| C6KET34O | CCC([O])C(=O)CC | InChI=1S/C6H11O2/c1-3-5(7)6(8)4-2/h5H,3-4H2,1-2H3 |  | C6H11O2 |
| C6KET35O | CC([O])CC(=O)CC | InChI=1S/C6H11O2/c1-3-6(8)4-5(2)7/h5H,3-4H2,1-2H3 | C6H11O2 |
| C6KET36O | C([O])CCC(=O)CC | InChI=1S/C6H11O2/c1-2-6(8)4-3-5-7/h2-5H2,1H3 |  | C6H11O2 |
| C6H10D13 | C=CC=CCC | InChI=1S/C6H10/c1-3-5-6-4-2/h3,5-6H,1,4H2,2H3 |  | C6H10 |
| C6H10D24 | CC=CC=CC | InChI=1S/C6H10/c1-3-5-6-4-2/h3-6H,1-2H3 |  | C6H10 |
| C6H12OOH1-2O | C(OO)C([O])CCCC | InChI=1S/C6H13O3/c1-2-3-4-6(7)5-9-8/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OOH1-3O | C(OO)CC([O])CCC | InChI=1S/C6H13O3/c1-2-3-6(7)4-5-9-8/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OOH1-4O | C(OO)CCC([O])CC | InChI=1S/C6H13O3/c1-2-6(7)4-3-5-9-8/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OOH1-5O | C(OO)CCCC([O])C | InChI=1S/C6H13O3/c1-6(7)4-2-3-5-9-8/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OOH2-1O | C([O])C(OO)CCCC | InChI=1S/C6H13O3/c1-2-3-4-6(5-7)9-8/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OOH2-3O | CC(OO)C([O])CCC | InChI=1S/C6H13O3/c1-3-4-6(7)5(2)9-8/h5-6,8H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OOH2-4O | CC(OO)CC([O])CC | InChI=1S/C6H13O3/c1-3-6(7)4-5(2)9-8/h5-6,8H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OOH2-5O | CC(OO)CCC([O])C | InChI=1S/C6H13O3/c1-5(7)3-4-6(2)9-8/h5-6,8H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OOH2-6O | CC(OO)CCCC([O]) | InChI=1S/C6H13O3/c1-6(9-8)4-2-3-5-7/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OOH3-1O | C([O])CC(OO)CCC | InChI=1S/C6H13O3/c1-2-3-6(9-8)4-5-7/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| C6H12OOH3-2O | CC([O])C(OO)CCC | InChI=1S/C6H13O3/c1-3-4-6(9-8)5(2)7/h5-6,8H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OOH3-4O | CCC(OO)C([O])CC | InChI=1S/C6H13O3/c1-3-5(7)6(4-2)9-8/h5-6,8H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OOH3-5O | CCC(OO)CC([O])C | InChI=1S/C6H13O3/c1-3-6(9-8)4-5(2)7/h5-6,8H,3-4H2,1-2H3 |  | C6H13O3 |
| C6H12OOH3-6O | CCC(OO)CCC([O]) | InChI=1S/C6H13O3/c1-2-6(9-8)4-3-5-7/h6,8H,2-5H2,1H3 |  | C6H13O3 |
| NC5H11CHO | CCCCCC=O | InChI=1S/C6H12O/c1-2-3-4-5-6-7/h6H,2-5H2,1H3 |  | C6H12O |
| C6Y2 | CC(=O)CCCC | InChI=1S/C6H12O/c1-3-4-5-6(2)7/h3-5H2,1-2H3 |  | C6H12O |
| NC5H11CO | CCCCC[C]=O | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2-5H2,1H3 |  | C6H11O |
| NC5H10CHO-1 | CCCC[CH]C=O | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h5-6H,2-4H2,1H3 |  | C6H11O |
| NC5H10CHO-2 | CCC[CH]CC=O | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h4,6H,2-3,5H2,1H3 |  | C6H11O |
| NC5H10CHO-3 | CC[CH]CCC=O | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h3,6H,2,4-5H2,1H3 |  | C6H11O |
| NC5H10CHO-4 | C[CH]CCCC=O | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h2,6H,3-5H2,1H3 |  | C6H11O |
| NC5H10CHO-5 | [CH2]CCCCC=O | InChI=1S/C6H11O/c1-2-3-4-5-6-7/h6H,1-5H2 |  | C6H11O |
| CH3COOH | CC(=O)O | InChI=1S/C2H4O2/c1-2(3)4/h1H3,(H,3,4) |  | C2H4O2 |
| C2H5COOH | CCC(=O)O | InChI=1S/C3H6O2/c1-2-3(4)5/h2H2,1H3,(H,4,5) |  | C3H6O2 |
| I3C6 | CCC(C)CC | InChI=1S/C6H14/c1-4-6(3)5-2/h6H,4-5H2,1-3H3 |

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 | C6H14 |
| I3C6-1 | [CH2]CC(C)CC | InChI=1S/C6H13/c1-4-6(3)5-2/h6H,1,4-5H2,2-3H3 |  | C6H13 |
| I3C6-2 | C[CH]C(C)CC | InChI=1S/C6H13/c1-4-6(3)5-2/h4,6H,5H2,1-3H3 |  | C6H13 |
| I3C6-3 | CC[C](C)CC | InChI=1S/C6H13/c1-4-6(3)5-2/h4-5H2,1-3H3 |  | C6H13 |
| I3C6-4 | CCC([CH2])CC | InChI=1S/C6H13/c1-4-6(3)5-2/h6H,3-5H2,1-2H3 |  | C6H13 |
| I3C6D1 | C=CC(C)CC | InChI=1S/C6H12/c1-4-6(3)5-2/h4,6H,1,5H2,2-3H3 |  | C6H12 |
| I3C6D2 | CC=C(C)CC | InChI=1S/C6H12/c1-4-6(3)5-2/h4H,5H2,1-3H3 |  | C6H12 |
| I3C6D3 | CCC(=C)CC | InChI=1S/C6H12/c1-4-6(3)5-2/h3-5H2,1-2H3 |  | C6H12 |
| I3C6D1-3 | C=C[C](C)CC | InChI=1S/C6H11/c1-4-6(3)5-2/h4H,1,5H2,2-3H3 |  | C6H11 |
| I3C6D1-4 | C=CC([CH2])CC | InChI=1S/C6H11/c1-4-6(3)5-2/h4,6H,1,3,5H2,2H3 |  | C6H11 |
| I3C6D1-5 | C=CC(C)[CH]C | InChI=1S/C6H11/c1-4-6(3)5-2/h4-6H,1H2,2-3H3 |  | C6H11 |
| I3C6D1-6 | C=CC(C)C[CH2] | InChI=1S/C6H11/c1-4-6(3)5-2/h4,6H,1-2,5H2,3H3 |  | C6H11 |
| I3C6D2-5 | CC=C(C)[CH]C | InChI=1S/C6H11/c1-4-6(3)5-2/h4-5H,1-3H3 |  | C6H11 |
| I3C6D2-6 | CC=C(C)C[CH2] | InChI=1S/C6H11/c1-4-6(3)5-2/h5H,1,4H2,2-3H3 |  | C6H11 |
| I3C6D3-1 | [CH2]CC(=C)CC | InChI=1S/C6H11/c1-4-6(3)5-2/h1,3-5H2,2H3 |  | C6H11 |
| I3C6D3-2 | C[CH]C(=C)CC | InChI=1S/C6H11/c1-4-6(3)5-2/h4H,3,5H2,1-2H3 |  | C6H11 |
| I3C6OH1-2J | C(O)[CH]C(C)CC | InChI=1S/C6H13O/c1-3-6(2)4-5-7/h4,6-7H,3,5H2,1-2H3 |  | C6H13O |
| I3C6OH2-1J | [CH2]C(O)C(C)CC | InChI=1S/C6H13O/c1-4-5(2)6(3)7/h5-7H,3-4H2,1-2H3 |  | C6H13O |
| I3C6OH2-3J | CC(O)[C](C)CC | InChI=1S/C6H13O/c1-4-5(2)6(3)7/h6-7H,4H2,1-3H3 |  | C6H13O |
| I3C6OH3-2J | C[CH]C(C)(O)CC | InChI=1S/C6H13O/c1-4-6(3,7)5-2/h4,7H,5H2,1-3H3 |  | C6H13O |
| I3C6OH3-4J | CCC([CH2])(O)CC | InChI=1S/C6H13O/c1-4-6(3,7)5-2/h7H,3-5H2,1-2H3 |  | C6H13O |
| I3C6OH4-3J | CC[C](CO)CC | InChI=1S/C6H13O/c1-3-6(4-2)5-7/h7H,3-5H2,1-2H3 |  | C6H13O |
| I3C6OH1-2O2 | C(O)C(O[O])C(C)CC | InChI=1S/C6H13O3/c1-3-5(2)6(4-7)9-8/h5-7H,3-4H2,1-2H3 |  | C6H13O3 |
| I3C6OH2-1O2 | C(O[O])C(O)C(C)CC | InChI=1S/C6H13O3/c1-3-5(2)6(7)4-9-8/h5-7H,3-4H2,1-2H3 |  | C6H13O3 |
| I3C6OH2-3O2 | CC(O)C(C)(O[O])CC | InChI=1S/C6H13O3/c1-4-6(3,9-8)5(2)7/h5,7H,4H2,1-3H3 |  | C6H13O3 |
| I3C6OH3-2O2 | CC(O[O])C(C)(O)CC | InChI=1S/C6H13O3/c1-4-6(3,7)5(2)9-8/h5,7H,4H2,1-3H3 |  | C6H13O3 |
| I3C6OH3-4O2 | CCC(CO[O])(O)CC | InChI=1S/C6H13O3/c1-3-6(7,4-2)5-9-8/h7H,3-5H2,1-2H3 |  | C6H13O3 |
| I3C6OH4-3O2 | CCC(CO)(O[O])CC | InChI=1S/C6H13O3/c1-3-6(4-2,5-7)9-8/h7H,3-5H2,1-2H3 |  | C6H13O3 |
| I3C6D1-3O | C=CC(C)(O)CC | InChI=1S/C6H12O/c1-4-6(3,7)5-2/h4,7H,1,5H2,2-3H3 |  | C6H12O |
| I3C6D1-4O | C=CC(CO)CC | InChI=1S/C6H12O/c1-3-6(4-2)5-7/h3,6-7H,1,4-5H2,2H3 |  | C6H12O |
| I3C6D1-5O | C=CC(C)C(O)C | InChI=1S/C6H12O/c1-4-5(2)6(3)7/h4-7H,1H2,2-3H3 |  | C6H12O |
| I3C6D1-6O | C=CC(C)CC(O) | InChI=1S/C6H12O/c1-3-6(2)4-5-7/h3,6-7H,1,4-5H2,2H3 |  | C6H12O |
| I3C6D2-5O | CC=C(C)C(O)C | InChI=1S/C6H12O/c1-4-5(2)6(3)7/h4,6-7H,1-3H3 |  | C6H12O |
| I3C6D2-6O | CC=C(C)CC(O) | InChI=1S/C6H12O/c1-3-6(2)4-5-7/h3,7H,4-5H2,1-2H3 |  | C6H12O |
| I3C6D3-1O | CCC(=C)CC(O) | InChI=1S/C6H12O/c1-3-6(2)4-5-7/h7H,2-5H2,1H3 |  | C6H12O |
| I3C6D3-2O | CCC(=C)C(O)C | InChI=1S/C6H12O/c1-4-5(2)6(3)7/h6-7H,2,4H2,1,3H3 |  | C6H12O |
| I3C6-1OOH | C(OO)CC(C)CC | InChI=1S/C6H14O2/c1-3-6(2)4-5-8-7/h6-7H,3-5H2,1-2H3 |  | C6H14O2 |
| I3C6-1O2 | C(O[O])CC(C)CC | InChI=1S/C6H13O2/c1-3-6(2)4-5-8-7/h6H,3-5H2,1-2H3 |  | C6H13O2 |
| I3C6-2OOH | CC(OO)C(C)CC | InChI=1S/C6H14O2/c1-4-5(2)6(3)8-7/h5-7H,4H2,1-3H3 |  | C6H14O2 |
| I3C6-2O2 | CC(O[O])C(C)CC | InChI=1S/C6H13O2/c1-4-5(2)6(3)8-7/h5-6H,4H2,1-3H3 |  | C6H13O2 |
| I3C6-3OOH | CCC(C)(OO)CC | InChI=1S/C6H14O2/c1-4-6(3,5-2)8-7/h7H,4-5H2,1-3H3 |  | C6H14O2 |
| I3C6-3O2 | CCC(C)(O[O])CC | InChI=1S/C6H13O2/c1-4-6(3,5-2)8-7/h4-5H2,1-3H3 |  | C6H13O2 |
| I3C6-4OOH | CCC(COO)CC | InChI=1S/C6H14O2/c1-3-6(4-2)5-8-7/h6-7H,3-5H2,1-2H3 |  | C6H14O2 |
| I3C6-4O2 | CCC(CO[O])CC | InChI=1S/C6H13O2/c1-3-6(4-2)5-8-7/h6H,3-5H2,1-2H3 |  | C6H13O2 |
| I3C6-1O | C([O])CC(C)CC | InChI=1S/C6H13O/c1-3-6(2)4-5-7/h6H,3-5H2,1-2H3 |  | C6H13O |
| I3C6-2O | CC([O])C(C)CC | InChI=1S/C6H13O/c1-4-5(2)6(3)7/h5-6H,4H2,1-3H3 |  | C6H13O |
| I3C6-3O | CCC(C)([O])CC | InChI=1S/C6H13O/c1-4-6(3,7)5-2/h4-5H2,1-3H3 |  | C6H13O |
| I3C6-4O | CCC(C[O])CC | InChI=1S/C6H13O/c1-3-6(4-2)5-7/h6H,3-5H2,1-2H3 |  | C6H13O |
| I3C6OOH1-2 | C(OO)[CH]C(C)CC | InChI=1S/C6H13O2/c1-3-6(2)4-5-8-7/h4,6-7H,3,5H2,1-2H3 |  | C6H13O2 |
| I3C6OOH1-3 | C(OO)C[C](C)CC | InChI=1S/C6H13O2/c1-3-6(2)4-5-8-7/h7H,3-5H2,1-2H3 |  | C6H13O2 |
| I3C6OOH1-4 | C(OO)CC([CH2])CC | InChI=1S/C6H13O2/c1-3-6(2)4-5-8-7/h6-7H,2-5H2,1H3 |  | C6H13O2 |
| I3C6OOH1-5 | C(OO)CC(C)[CH]C | InChI=1S/C6H13O2/c1-3-6(2)4-5-8-7/h3,6-7H,4-5H2,1-2H3 |  | C6H13O2 |
| I3C6OOH1-6 | C(OO)CC(C)C[CH2] | InChI=1S/C6H13O2/c1-3-6(2)4-5-8-7/h6-7H,1,3-5H2,2H3 |  | C6H13O2 |
| I3C6OOH2-1 | [CH2]C(OO)C(C)CC | InChI=1S/C6H13O2/c1-4-5(2)6(3)8-7/h5-7H,3-4H2,1-2H3 |  | C6H13O2 |
| I3C6OOH2-3 | CC(OO)[C](C)CC | InChI=1S/C6H13O2/c1-4-5(2)6(3)8-7/h6-7H,4H2,1-3H3 |  | C6H13O2 |
| I3C6OOH2-4 | CC(OO)C([CH2])CC | InChI=1S/C6H13O2/c1-4-5(2)6(3)8-7/h5-7H,2,4H2,1,3H3 |  | C6H13O2 |
| I3C6OOH2-5 | CC(OO)C(C)[CH]C | InChI=1S/C6H13O2/c1-4-5(2)6(3)8-7/h4-7H,1-3H3 |  | C6H13O2 |
| I3C6OOH2-6 | CC(OO)C(C)C[CH2] | InChI=1S/C6H13O2/c1-4-5(2)6(3)8-7/h5-7H,1,4H2,2-3H3 |  | C6H13O2 |
| I3C6OOH3-1 | [CH2]CC(C)(OO)CC | InChI=1S/C6H13O2/c1-4-6(3,5-2)8-7/h7H,1,4-5H2,2-3H3 |  | C6H13O2 |
| I3C6OOH3-2 | C[CH]C(C)(OO)CC | InChI=1S/C6H13O2/c1-4-6(3,5-2)8-7/h4,7H,5H2,1-3H3 |  | C6H13O2 |
| I3C6OOH3-4 | CCC([CH2])(OO)CC | InChI=1S/C6H13O2/c1-4-6(3,5-2)8-7/h7H,3-5H2,1-2H3 |  | C6H13O2 |
| I3C6OOH4-1 | [CH2]CC(COO)CC | InChI=1S/C6H13O2/c1-3-6(4-2)5-8-7/h6-7H,1,3-5H2,2H3 |  | C6H13O2 |
| I3C6OOH4-2 | C[CH]C(COO)CC | InChI=1S/C6H13O2/c1-3-6(4-2)5-8-7/h3,6-7H,4-5H2,1-2H3 |  | C6H13O2 |
| I3C6OOH4-3 | CC[C](COO)CC | InChI=1S/C6H13O2/c1-3-6(4-2)5-8-7/h7H,3-5H2,1-2H3 |  | C6H13O2 |
| I3C6O1-2 | C1C(O1)C(C)CC | InChI=1S/C6H12O/c1-3-5(2)6-4-7-6/h5-6H,3-4H2,1-2H3 |  | C6H12O |
| I3C6O1-3 | C1CC(C)(O1)CC | InChI=1S/C6H12O/c1-3-6(2)4-5-7-6/h3-5H2,1-2H3 |  | C6H12O |
| I3C6O1-4 | C1CC(CO1)CC | InChI=1S/C6H12O/c1-2-6-3-4-7-5-6/h6H,2-5H2,1H3 |  | C6H12O |
| I3C6O1-5 | C1CC(C)C(O1)C | InChI=1S/C6H12O/c1-5-3-4-7-6(5)2/h5-6H,3-4H2,1-2H3 |  | C6H12O |
| I3C6O1-6 | C1CC(C)CC(O1) | InChI=1S/C6H12O/c1-6-2-4-7-5-3-6/h6H,2-5H2,1H3 |  | C6H12O |
| I3C6O2-3 | CC1C(C)(O1)CC | InChI=1S/C6H12O/c1-4-6(3)5(2)7-6/h5H,4H2,1-3H3 |  | C6H12O |
| I3C6O2-4 | CC1C(CO1)CC | InChI=1S/C6H12O/c1-3-6-4-7-5(6)2/h5-6H,3-4H2,1-2H3 |  | C6H12O |
| I3C6O2-5 | CC1C(C)C(O1)C | InChI=1S/C6H12O/c1-4-5(2)7-6(4)3/h4-6H,1-3H3 |  | C6H12O |
| I3C6O3-4 | CCC1(CO1)CC | InChI=1S/C6H12O/c1-3-6(4-2)5-7-6/h3-5H2,1-2H3 |  | C6H12O |
| I3C6OOH1-2O2 | C(OO)C(O[O])C(C)CC | InChI=1S/C6H13O4/c1-3-5(2)6(10-8)4-9-7/h5-7H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6OOH1-3O2 | C(OO)CC(C)(O[O])CC | InChI=1S/C6H13O4/c1-3-6(2,10-8)4-5-9-7/h7H,3-5H2,1-2H3 |  | C6H13O4 |
| I3C6OOH1-4O2 | C(OO)CC(CO[O])CC | InChI=1S/C6H13O4/c1-2-6(5-10-8)3-4-9-7/h6-7H,2-5H2,1H3 |  | C6H13O4 |
| I3C6OOH1-5O2 | C(OO)CC(C)C(O[O])C | InChI=1S/C6H13O4/c1-5(3-4-9-7)6(2)10-8/h5-7H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6OOH1-6O2 | C(OO)CC(C)CC(O[O]) | InChI=1S/C6H13O4/c1-6(2-4-9-7)3-5-10-8/h6-7H,2-5H2,1H3 |  | C6H13O4 |
| I3C6OOH2-1O2 | CCC(C)C(OO)C(O[O]) | InChI=1S/C6H13O4/c1-3-5(2)6(10-8)4-9-7/h5-6,8H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6OOH2-3O2 | CCC(C)(O[O])C(OO)C | InChI=1S/C6H13O4/c1-4-6(3,10-8)5(2)9-7/h5,7H,4H2,1-3H3 |  | C6H13O4 |
| I3C6OOH2-4O2 | CC(OO)C(CO[O])CC | InChI=1S/C6H13O4/c1-3-6(4-9-7)5(2)10-8/h5-6,8H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6OOH2-5O2 | CC(OO)C(C)C(O[O])C | InChI=1S/C6H13O4/c1-4(5(2)9-7)6(3)10-8/h4-7H,1-3H3 |  | C6H13O4 |
| I3C6OOH2-6O2 | CC(OO)C(C)CC(O[O]) | InChI=1S/C6H13O4/c1-5(3-4-9-7)6(2)10-8/h5-6,8H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6OOH3-1O2 | CCC(C)(OO)CC(O[O]) | InChI=1S/C6H13O4/c1-3-6(2,10-8)4-5-9-7/h8H,3-5H2,1-2H3 |  | C6H13O4 |
| I3C6OOH3-2O2 | CCC(C)(OO)C(O[O])C | InChI=1S/C6H13O4/c1-4-6(3,10-8)5(2)9-7/h5,8H,4H2,1-3H3 |  | C6H13O4 |
| I3C6OOH3-4O2 | CCC(CO[O])(OO)CC | InChI=1S/C6H13O4/c1-3-6(4-2,10-8)5-9-7/h8H,3-5H2,1-2H3 |  | C6H13O4 |
| I3C6OOH4-1O2 | CCC(COO)CC(O[O]) | InChI=1S/C6H13O4/c1-2-6(5-10-8)3-4-9-7/h6,8H,2-5H2,1H3 |  | C6H13O4 |
| I3C6OOH4-2O2 | CCC(COO)C(O[O])C | InChI=1S/C6H13O4/c1-3-6(4-9-7)5(2)10-8/h5-7H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6OOH4-3O2 | CCC(COO)(O[O])CC | InChI=1S/C6H13O4/c1-3-6(4-2,10-8)5-9-7/h7H,3-5H2,1-2H3 |  | C6H13O4 |
| I3C6KET1-2 | C(=O)C(OO)C(C)CC | InChI=1S/C6H12O3/c1-3-5(2)6(4-7)9-8/h4-6,8H,3H2,1-2H3 |  | C6H12O3 |
| I3C6KET1-3 | C(=O)CC(C)(OO)CC | InChI=1S/C6H12O3/c1-3-6(2,9-8)4-5-7/h5,8H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6KET1-4 | C(=O)CC(COO)CC | InChI=1S/C6H12O3/c1-2-6(3-4-7)5-9-8/h4,6,8H,2-3,5H2,1H3 |  | C6H12O3 |
| I3C6KET1-5 | C(=O)CC(C)C(OO)C | InChI=1S/C6H12O3/c1-5(3-4-7)6(2)9-8/h4-6,8H,3H2,1-2H3 |  | C6H12O3 |
| I3C6KET1-6 | C(=O)CC(C)CC(OO) | InChI=1S/C6H12O3/c1-6(2-4-7)3-5-9-8/h4,6,8H,2-3,5H2,1H3 |  | C6H12O3 |
| I3C6KET2-1 | CCC(C)C(=O)C(OO) | InChI=1S/C6H12O3/c1-3-5(2)6(7)4-9-8/h5,8H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6KET2-3 | CCC(C)(OO)C(=O)C | InChI=1S/C6H12O3/c1-4-6(3,9-8)5(2)7/h8H,4H2,1-3H3 |  | C6H12O3 |
| I3C6KET2-4 | CCC(COO)C(=O)C | InChI=1S/C6H12O3/c1-3-6(4-9-8)5(2)7/h6,8H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6KET2-5 | CC(OO)C(C)C(=O)C | InChI=1S/C6H12O3/c1-4(5(2)7)6(3)9-8/h4,6,8H,1-3H3 |  | C6H12O3 |
| I3C6KET2-6 | C(OO)CC(C)C(=O)C | InChI=1S/C6H12O3/c1-5(6(2)7)3-4-9-8/h5,8H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6KET4-1 | C(OO)CC(C=O)CC | InChI=1S/C6H12O3/c1-2-6(5-7)3-4-9-8/h5-6,8H,2-4H2,1H3 |  | C6H12O3 |
| I3C6KET4-2 | CC(OO)C(C=O)CC | InChI=1S/C6H12O3/c1-3-6(4-7)5(2)9-8/h4-6,8H,3H2,1-2H3 |  | C6H12O3 |
| I3C6KET4-3 | CCC(C=O)(OO)CC | InChI=1S/C6H12O3/c1-3-6(4-2,5-7)9-8/h5,8H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6D1-3OOH | C=CC(C)(OO)CC | InChI=1S/C6H12O2/c1-4-6(3,5-2)8-7/h4,7H,1,5H2,2-3H3 |  | C6H12O2 |
| I3C6D1-4OOH | C=CC(COO)CC | InChI=1S/C6H12O2/c1-3-6(4-2)5-8-7/h3,6-7H,1,4-5H2,2H3 |  | C6H12O2 |
| I3C6D1-5OOH | C=CC(C)C(OO)C | InChI=1S/C6H12O2/c1-4-5(2)6(3)8-7/h4-7H,1H2,2-3H3 |  | C6H12O2 |
| I3C6D1-6OOH | C=CC(C)CC(OO) | InChI=1S/C6H12O2/c1-3-6(2)4-5-8-7/h3,6-7H,1,4-5H2,2H3 |  | C6H12O2 |
| I3C6D2-1OOH | C(OO)C=C(C)CC | InChI=1S/C6H12O2/c1-3-6(2)4-5-8-7/h4,7H,3,5H2,1-2H3 |  | C6H12O2 |
| I3C6D2-4OOH | CC=C(COO)CC | InChI=1S/C6H12O2/c1-3-6(4-2)5-8-7/h3,7H,4-5H2,1-2H3 |  | C6H12O2 |
| I3C6D2-5OOH | CC=C(C)C(OO)C | InChI=1S/C6H12O2/c1-4-5(2)6(3)8-7/h4,6-7H,1-3H3 |  | C6H12O2 |
| I3C6D2-6OOH | CC=C(C)CC(OO) | InChI=1S/C6H12O2/c1-3-6(2)4-5-8-7/h3,7H,4-5H2,1-2H3 |  | C6H12O2 |
| I3C6D3-1OOH | CCC(=C)CC(OO) | InChI=1S/C6H12O2/c1-3-6(2)4-5-8-7/h7H,2-5H2,1H3 |  | C6H12O2 |
| I3C6D3-2OOH | CCC(=C)C(OO)C | InChI=1S/C6H12O2/c1-4-5(2)6(3)8-7/h6-7H,2,4H2,1,3H3 |  | C6H12O2 |
| I3C6Q12-3 | CC[C](C)C(OO)C(OO) | InChI=1S/C6H13O4/c1-3-5(2)6(10-8)4-9-7/h6-8H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6Q12-4 | CCC([CH2])C(OO)C(OO) | InChI=1S/C6H13O4/c1-3-5(2)6(10-8)4-9-7/h5-8H,2-4H2,1H3 |  | C6H13O4 |
| I3C6Q12-5 | C[CH]C(C)C(OO)C(OO) | InChI=1S/C6H13O4/c1-3-5(2)6(10-8)4-9-7/h3,5-8H,4H2,1-2H3 |  | C6H13O4 |
| I3C6Q12-6 | [CH2]CC(C)C(OO)C(OO) | InChI=1S/C6H13O4/c1-3-5(2)6(10-8)4-9-7/h5-8H,1,3-4H2,2H3 |  | C6H13O4 |
| I3C6Q13-2 | CCC(C)(OO)[CH]C(OO) | InChI=1S/C6H13O4/c1-3-6(2,10-8)4-5-9-7/h4,7-8H,3,5H2,1-2H3 |  | C6H13O4 |
| I3C6Q13-4 | CCC([CH2])(OO)CC(OO) | InChI=1S/C6H13O4/c1-3-6(2,10-8)4-5-9-7/h7-8H,2-5H2,1H3 |  | C6H13O4 |
| I3C6Q13-5 | C[CH]C(C)(OO)CC(OO) | InChI=1S/C6H13O4/c1-3-6(2,10-8)4-5-9-7/h3,7-8H,4-5H2,1-2H3 |  | C6H13O4 |
| I3C6Q13-6 | [CH2]CC(C)(OO)CC(OO) | InChI=1S/C6H13O4/c1-3-6(2,10-8)4-5-9-7/h7-8H,1,3-5H2,2H3 |  | C6H13O4 |
| I3C6Q14-2 | CCC(COO)[CH]C(OO) | InChI=1S/C6H13O4/c1-2-6(5-10-8)3-4-9-7/h3,6-8H,2,4-5H2,1H3 |  | C6H13O4 |
| I3C6Q14-3 | CC[C](COO)CC(OO) | InChI=1S/C6H13O4/c1-2-6(5-10-8)3-4-9-7/h7-8H,2-5H2,1H3 |  | C6H13O4 |
| I3C6Q14-5 | C[CH]C(COO)CC(OO) | InChI=1S/C6H13O4/c1-2-6(5-10-8)3-4-9-7/h2,6-8H,3-5H2,1H3 |  | C6H13O4 |
| I3C6Q14-6 | [CH2]CC(COO)CC(OO) | InChI=1S/C6H13O4/c1-2-6(5-10-8)3-4-9-7/h6-8H,1-5H2 |  | C6H13O4 |
| I3C6Q15-2 | CC(OO)C(C)[CH]C(OO) | InChI=1S/C6H13O4/c1-5(3-4-9-7)6(2)10-8/h3,5-8H,4H2,1-2H3 |  | C6H13O4 |
| I3C6Q15-3 | CC(OO)[C](C)CC(OO) | InChI=1S/C6H13O4/c1-5(3-4-9-7)6(2)10-8/h6-8H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6Q15-4 | CC(OO)C([CH2])CC(OO) | InChI=1S/C6H13O4/c1-5(3-4-9-7)6(2)10-8/h5-8H,1,3-4H2,2H3 |  | C6H13O4 |
| I3C6Q15-6 | [CH2]C(OO)C(C)CC(OO) | InChI=1S/C6H13O4/c1-5(3-4-9-7)6(2)10-8/h5-8H,2-4H2,1H3 |  | C6H13O4 |
| I3C6Q16-2 | C(OO)CC(C)[CH]C(OO) | InChI=1S/C6H13O4/c1-6(2-4-9-7)3-5-10-8/h2,6-8H,3-5H2,1H3 |  | C6H13O4 |
| I3C6Q16-3 | C(OO)C[C](C)CC(OO) | InChI=1S/C6H13O4/c1-6(2-4-9-7)3-5-10-8/h7-8H,2-5H2,1H3 |  | C6H13O4 |
| I3C6Q16-4 | C(OO)CC([CH2])CC(OO) | InChI=1S/C6H13O4/c1-6(2-4-9-7)3-5-10-8/h6-8H,1-5H2 |  | C6H13O4 |
| I3C6Q23-1 | [CH2]C(OO)C(C)(OO)CC | InChI=1S/C6H13O4/c1-4-6(3,10-8)5(2)9-7/h5,7-8H,2,4H2,1,3H3 |  | C6H13O4 |
| I3C6Q23-4 | CC(OO)C([CH2])(OO)CC | InChI=1S/C6H13O4/c1-4-6(3,10-8)5(2)9-7/h5,7-8H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6Q23-5 | CC(OO)C(C)(OO)[CH]C | InChI=1S/C6H13O4/c1-4-6(3,10-8)5(2)9-7/h4-5,7-8H,1-3H3 |  | C6H13O4 |
| I3C6Q23-6 | CC(OO)C(C)(OO)C[CH2] | InChI=1S/C6H13O4/c1-4-6(3,10-8)5(2)9-7/h5,7-8H,1,4H2,2-3H3 |  | C6H13O4 |
| I3C6Q24-1 | [CH2]C(OO)C(COO)CC | InChI=1S/C6H13O4/c1-3-6(4-9-7)5(2)10-8/h5-8H,2-4H2,1H3 |  | C6H13O4 |
| I3C6Q24-3 | CC(OO)[C](COO)CC | InChI=1S/C6H13O4/c1-3-6(4-9-7)5(2)10-8/h5,7-8H,3-4H2,1-2H3 |  | C6H13O4 |
| I3C6Q24-5 | CC(OO)C(COO)[CH]C | InChI=1S/C6H13O4/c1-3-6(4-9-7)5(2)10-8/h3,5-8H,4H2,1-2H3 |  | C6H13O4 |
| I3C6Q24-6 | CC(OO)C(COO)C[CH2] | InChI=1S/C6H13O4/c1-3-6(4-9-7)5(2)10-8/h5-8H,1,3-4H2,2H3 |  | C6H13O4 |
| I3C6Q25-1 | CC(OO)C(C)C(OO)[CH2] | InChI=1S/C6H13O4/c1-4(5(2)9-7)6(3)10-8/h4-8H,2H2,1,3H3 |  | C6H13O4 |
| I3C6Q25-3 | CC(OO)[C](C)C(OO)C | InChI=1S/C6H13O4/c1-4(5(2)9-7)6(3)10-8/h5-8H,1-3H3 |  | C6H13O4 |
| I3C6Q25-4 | CC(OO)C([CH2])C(OO)C | InChI=1S/C6H13O4/c1-4(5(2)9-7)6(3)10-8/h4-8H,1H2,2-3H3 |  | C6H13O4 |
| I3C6Q34-1 | [CH2]CC(COO)(OO)CC | InChI=1S/C6H13O4/c1-3-6(4-2,10-8)5-9-7/h7-8H,1,3-5H2,2H3 |  | C6H13O4 |
| I3C6Q34-2 | C[CH]C(COO)(OO)CC | InChI=1S/C6H13O4/c1-3-6(4-2,10-8)5-9-7/h3,7-8H,4-5H2,1-2H3 |  | C6H13O4 |
| I3C6O12-3OOH | C1C(O1)C(C)(OO)CC | InChI=1S/C6H12O3/c1-3-6(2,9-7)5-4-8-5/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O12-4OOH | C1C(O1)C(COO)CC | InChI=1S/C6H12O3/c1-2-5(3-9-7)6-4-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O12-5OOH | C1C(O1)C(C)C(OO)C | InChI=1S/C6H12O3/c1-4(5(2)9-7)6-3-8-6/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| I3C6O12-6OOH | C1C(O1)C(C)CC(OO) | InChI=1S/C6H12O3/c1-5(2-3-9-7)6-4-8-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O13-2OOH | C1C(OO)C(C)(O1)CC | InChI=1S/C6H12O3/c1-3-6(2)5(9-7)4-8-6/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O13-4OOH | C1CC(COO)(O1)CC | InChI=1S/C6H12O3/c1-2-6(5-9-7)3-4-8-6/h7H,2-5H2,1H3 |  | C6H12O3 |
| I3C6O13-5OOH | C1CC(C)(O1)C(OO)C | InChI=1S/C6H12O3/c1-5(9-7)6(2)3-4-8-6/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O13-6OOH | C1CC(C)(O1)CC(OO) | InChI=1S/C6H12O3/c1-6(2-4-8-6)3-5-9-7/h7H,2-5H2,1H3 |  | C6H12O3 |
| I3C6O14-2OOH | C1C(OO)C(CO1)CC | InChI=1S/C6H12O3/c1-2-5-3-8-4-6(5)9-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O14-3OOH | C1CC(CO1)(OO)CC | InChI=1S/C6H12O3/c1-2-6(9-7)3-4-8-5-6/h7H,2-5H2,1H3 |  | C6H12O3 |
| I3C6O14-5OOH | C1CC(CO1)C(OO)C | InChI=1S/C6H12O3/c1-5(9-7)6-2-3-8-4-6/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O14-6OOH | C1CC(CO1)CC(OO) | InChI=1S/C6H12O3/c7-9-4-2-6-1-3-8-5-6/h6-7H,1-5H2 |  | C6H12O3 |
| I3C6O15-2OOH | C1C(OO)C(C)C(O1)C | InChI=1S/C6H12O3/c1-4-5(2)8-3-6(4)9-7/h4-7H,3H2,1-2H3 | C6H12O3 |
| I3C6O15-3OOH | C1CC(C)(OO)C(O1)C | InChI=1S/C6H12O3/c1-5-6(2,9-7)3-4-8-5/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O15-4OOH | C1CC(COO)C(O1)C | InChI=1S/C6H12O3/c1-5-6(4-9-7)2-3-8-5/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O15-6OOH | C1CC(C)C(O1)C(OO) | InChI=1S/C6H12O3/c1-5-2-3-8-6(5)4-9-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O16-2OOH | C1C(OO)C(C)CC(O1) | InChI=1S/C6H12O3/c1-5-2-3-8-4-6(5)9-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O16-3OOH | C1CC(C)(OO)CC(O1) | InChI=1S/C6H12O3/c1-6(9-7)2-4-8-5-3-6/h7H,2-5H2,1H3 |  | C6H12O3 |
| I3C6O16-4OOH | C1CC(COO)CC(O1) | InChI=1S/C6H12O3/c7-9-5-6-1-3-8-4-2-6/h6-7H,1-5H2 |  | C6H12O3 |
| I3C6O23-1OOH | C(OO)C1C(C)(O1)CC | InChI=1S/C6H12O3/c1-3-6(2)5(9-6)4-8-7/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O23-4OOH | CC1C(COO)(O1)CC | InChI=1S/C6H12O3/c1-3-6(4-8-7)5(2)9-6/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O23-5OOH | CC1C(C)(O1)C(OO)C | InChI=1S/C6H12O3/c1-4-6(3,8-4)5(2)9-7/h4-5,7H,1-3H3 |  | C6H12O3 |
| I3C6O23-6OOH | CC1C(C)(O1)CC(OO) | InChI=1S/C6H12O3/c1-5-6(2,9-5)3-4-8-7/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O24-1OOH | C(OO)C1C(CO1)CC | InChI=1S/C6H12O3/c1-2-5-3-8-6(5)4-9-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O24-3OOH | CC1C(CO1)(OO)CC | InChI=1S/C6H12O3/c1-3-6(9-7)4-8-5(6)2/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| I3C6O24-5OOH | CC1C(CO1)C(OO)C | InChI=1S/C6H12O3/c1-4-6(3-8-4)5(2)9-7/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| I3C6O24-6OOH | CC1C(CO1)CC(OO) | InChI=1S/C6H12O3/c1-5-6(4-8-5)2-3-9-7/h5-7H,2-4H2,1H3 |  | C6H12O3 |
| I3C6O25-1OOH | CC1C(C)C(O1)C(OO) | InChI=1S/C6H12O3/c1-4-5(2)9-6(4)3-8-7/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| I3C6O25-3OOH | CC1C(C)(OO)C(O1)C | InChI=1S/C6H12O3/c1-4-6(3,9-7)5(2)8-4/h4-5,7H,1-3H3 |  | C6H12O3 |
| I3C6O25-4OOH | CC1C(COO)C(O1)C | InChI=1S/C6H12O3/c1-4-6(3-8-7)5(2)9-4/h4-7H,3H2,1-2H3 |  | C6H12O3 |
| I3C6O34-1OOH | C(OO)CC1(CO1)CC | InChI=1S/C6H12O3/c1-2-6(5-8-6)3-4-9-7/h7H,2-5H2,1H3 |  | C6H12O3 |
| I3C6O34-2OOH | CC(OO)C1(CO1)CC | InChI=1S/C6H12O3/c1-3-6(4-8-6)5(2)9-7/h5,7H,3-4H2,1-2H3 |  | C6H12O3 |
| IC4H8CHO-I | CC([CH2])CC=O | InChI=1S/C5H9O/c1-5(2)3-4-6/h4-5H,1,3H2,2H3 |  | C5H9O |
| IC5Y3-1J | [CH2]C(C)C(=O)C | InChI=1S/C5H9O/c1-4(2)5(3)6/h4H,1H2,2-3H3 |  | C5H9O |
| C5H9O2-1 | CCC=CC([O]) | InChI=1S/C5H9O/c1-2-3-4-5-6/h3-4H,2,5H2,1H3 |  | C5H9O |
| IC5O34-1J | CC([CH2])C1C(O1) | InChI=1S/C5H9O/c1-4(2)5-3-6-5/h4-5H,1,3H2,2H3 |  | C5H9O |
| C5Y2-3J | CC(=O)[CH]CC | InChI=1S/C5H9O/c1-3-4-5(2)6/h4H,3H2,1-2H3 |  | C5H9O |
| C5H9O15-3 | C1C[CH]CC(O1) | InChI=1S/C5H9O/c1-2-4-6-5-3-1/h1H,2-5H2 |  | C5H9O |
| AC5H9O-D | CC(=C)C[CH]C | InChI=1S/C6H11/c1-4-5-6(2)3/h4H,2,5H2,1,3H3 |  | C6H11 |
| IC5D1Y3 | CC(=C)C(=O)CC | InChI=1S/C6H10O/c1-4-6(7)5(2)3/h2,4H2,1,3H3 |  | C6H10O |
| SC4H9CHO | CC(C=O)CC | InChI=1S/C5H10O/c1-3-5(2)4-6/h4-5H,3H2,1-2H3 |  | C5H10O |
| SC4H9CO | CC([C]=O)CC | InChI=1S/C5H9O/c1-3-5(2)4-6/h5H,3H2,1-2H3 |  | C5H9O |
| SC4H8CHO-1 | [CH2]C(C=O)CC | InChI=1S/C5H9O/c1-3-5(2)4-6/h4-5H,2-3H2,1H3 |  | C5H9O |
| SC4H8CHO-2 | C[C](C=O)CC | InChI=1S/C5H9O/c1-3-5(2)4-6/h4H,3H2,1-2H3 |  | C5H9O |
| SC4H8CHO-3 | CC(C=O)[CH]C | InChI=1S/C5H9O/c1-3-5(2)4-6/h3-5H,1-2H3 |  | C5H9O |
| SC4H8CHO-4 | CC(C=O)C[CH2] | InChI=1S/C5H9O/c1-3-5(2)4-6/h4-5H,1,3H2,2H3 |  | C5H9O |
| C5Y3 | CCC(=O)CC | InChI=1S/C5H10O/c1-3-5(6)4-2/h3-4H2,1-2H3 |  | C5H10O |
| C5Y3-2J | C[CH]C(=O)CC | InChI=1S/C5H9O/c1-3-5(6)4-2/h3H,4H2,1-2H3 |  | C5H9O |
| IC5H8D13 | CC(=C)C=C | InChI=1S/C5H8/c1-4-5(2)3/h4H,1-2H2,3H3 |  | C5H8 |
| IC5H8D13-1A | [CH2]C(=C)C=C | InChI=1S/C5H7/c1-4-5(2)3/h4H,1-3H2 |  | C5H7 |
| I3C6KET1-2O | C(=O)C([O])C(C)CC | InChI=1S/C6H11O2/c1-3-5(2)6(8)4-7/h4-6H,3H2,1-2H3 |  | C6H11O2 |
| I3C6KET1-3O | C(=O)CC(C)([O])CC | InChI=1S/C6H11O2/c1-3-6(2,8)4-5-7/h5H,3-4H2,1-2H3 |  | C6H11O2 |
| I3C6KET1-4O | C(=O)CC(C[O])CC | InChI=1S/C6H11O2/c1-2-6(5-8)3-4-7/h4,6H,2-3,5H2,1H3 |  | C6H11O2 |
| I3C6KET1-5O | C(=O)CC(C)C([O])C | InChI=1S/C6H11O2/c1-5(3-4-7)6(2)8/h4-6H,3H2,1-2H3 |  | C6H11O2 |
| I3C6KET1-6O | C(=O)CC(C)CC([O]) | InChI=1S/C6H11O2/c1-6(2-4-7)3-5-8/h4,6H,2-3,5H2,1H3 |  | C6H11O2 |
| I3C6KET2-1O | CCC(C)C(=O)C([O]) | InChI=1S/C6H11O2/c1-3-5(2)6(8)4-7/h5H,3-4H2,1-2H3 |  | C6H11O2 |
| I3C6KET2-3O | CCC(C)([O])C(=O)C | InChI=1S/C6H11O2/c1-4-6(3,8)5(2)7/h4H2,1-3H3 |  | C6H11O2 |
| I3C6KET2-4O | CCC(C[O])C(=O)C | InChI=1S/C6H11O2/c1-3-6(4-7)5(2)8/h6H,3-4H2,1-2H3 |  | C6H11O2 |
| I3C6KET2-5O | CC([O])C(C)C(=O)C | InChI=1S/C6H11O2/c1-4(5(2)7)6(3)8/h4-5H,1-3H3 |  | C6H11O2 |
| I3C6KET2-6O | C([O])CC(C)C(=O)C | InChI=1S/C6H11O2/c1-5(3-4-7)6(2)8/h5H,3-4H2,1-2H3 |  | C6H11O2 |
| I3C6KET4-1O | C([O])CC(C=O)CC | InChI=1S/C6H11O2/c1-2-6(5-8)3-4-7/h5-6H,2-4H2,1H3 |  | C6H11O2 |
| I3C6KET4-2O | CC([O])C(C=O)CC | InChI=1S/C6H11O2/c1-3-6(4-7)5(2)8/h4-6H,3H2,1-2H3 |  | C6H11O2 |
| I3C6KET4-3O | CCC(C=O)([O])CC | InChI=1S/C6H11O2/c1-3-6(8,4-2)5-7/h5H,3-4H2,1-2H3 |  | C6H11O2 |