

d-Gluconic acid, 2,3,4,6-tetra-O-methyl-, «delta»-lactone

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|-----------------------------|---|
| Other names: | D-(+)-Gluconic acid «delta»-lactone, tetramethyl ether |
| Inchi: | InChI=1S/C10H18O6/c1-12-5-6-7(13-2)8(14-3)9(15-4)10(11)16-6/h6-9H,5H2,1-4H3 |
| InchiKey: | VKQXSSPDIRLBRM-UHFFFAOYSA-N |
| Formula: | C10H18O6 |
| SMILES: | COCC1OC(=O)C(OC)C(OC)C1OC |
| Mol. weight [g/mol]: | 234.25 |
| CAS: | 35510-38-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| gf | -594.07 | kJ/mol | Joback Method |
| hf | -1055.01 | kJ/mol | Joback Method |
| hfus | 28.95 | kJ/mol | Joback Method |
| hvap | 55.75 | kJ/mol | Joback Method |
| log10ws | 0.44 | | Crippen Method |
| logp | -0.397 | | Crippen Method |
| mcvol | 171.820 | ml/mol | McGowan Method |
| pc | 2237.64 | kPa | Joback Method |
| rinpol | 1559.20 | | NIST Webbook |
| tb | 618.19 | K | Joback Method |
| tc | 821.19 | K | Joback Method |
| tf | 380.83 | K | Joback Method |
| vc | 0.625 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 484.81 | J/molxK | 618.19 | Joback Method |
| cpg | 503.03 | J/molxK | 652.02 | Joback Method |
| cpg | 520.48 | J/molxK | 685.86 | Joback Method |
| cpg | 537.09 | J/molxK | 719.69 | Joback Method |
| cpg | 552.79 | J/molxK | 753.52 | Joback Method |
| cpg | 567.50 | J/molxK | 787.36 | Joback Method |
| cpg | 581.16 | J/molxK | 821.19 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C35510384&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvp: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinp: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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