

D-fructopyranose, 2,3:5,6-di-o-isopropylidene-

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H20O6/c1-10(2)15-6-12(18-10)9(13)8-7(5-14-12)16-11(3,4)17-8/h7-9,13H, |
| InchiKey: | NFH XOQDPQIQPKT-JACXVAGASA-N |
| Formula: | C12H20O6 |
| SMILES: | CC1(C)OC2COC3(COC(C)(C)O3)C(O)C2O1 |
| Mol. weight [g/mol]: | 260.28 |
| CAS: | 15080-25-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -423.01 | kJ/mol | Joback Method |
| hf | -924.78 | kJ/mol | Joback Method |
| hfus | 41.14 | kJ/mol | Joback Method |
| hvap | 77.58 | kJ/mol | Joback Method |
| log10ws | -1.39 | | Crippen Method |
| logp | 0.377 | | Crippen Method |
| mcvol | 182.580 | ml/mol | McGowan Method |
| pc | 3096.73 | kPa | Joback Method |
| tb | 724.90 | K | Joback Method |
| tc | 951.13 | K | Joback Method |
| tf | 517.39 | K | Joback Method |
| vc | 0.661 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 602.64 | J/molxK | 724.90 | Joback Method |
| cpg | 620.05 | J/molxK | 762.61 | Joback Method |
| cpg | 637.43 | J/molxK | 800.31 | Joback Method |
| cpg | 655.11 | J/molxK | 838.02 | Joback Method |
| cpg | 673.46 | J/molxK | 875.72 | Joback Method |
| cpg | 692.82 | J/molxK | 913.43 | Joback Method |
| cpg | 713.54 | J/molxK | 951.13 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=C15080258&Units=SI |

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 |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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