

Adonitol, pentamethyl ether

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|-----------------------------|---|
| Inchi: | InChI=1S/C10H22O5/c1-11-6-8(13-3)10(15-5)9(14-4)7-12-2/h8-10H,6-7H2,1-5H3 |
| InchiKey: | UKACKIRJWDAFEZ-UHFFFAOYSA-N |
| Formula: | C10H22O5 |
| SMILES: | COCC(OC)C(OC)C(COC)OC |
| Mol. weight [g/mol]: | 222.28 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -499.00 | kJ/mol | Joback Method |
| hf | -926.67 | kJ/mol | Joback Method |
| hfus | 17.03 | kJ/mol | Joback Method |
| hvap | 48.74 | kJ/mol | Joback Method |
| log10ws | 0.22 | | Crippen Method |
| logp | 0.324 | | Crippen Method |
| mcvol | 181.110 | ml/mol | McGowan Method |
| pc | 1994.77 | kPa | Joback Method |
| rinsol | 1277.80 | | NIST Webbook |
| tb | 538.98 | K | Joback Method |
| tc | 710.38 | K | Joback Method |
| tf | 268.61 | K | Joback Method |
| vc | 0.667 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 450.67 | J/molxK | 538.98 | Joback Method |
| cpg | 521.81 | J/molxK | 681.81 | Joback Method |
| cpg | 508.52 | J/molxK | 653.24 | Joback Method |
| cpg | 494.75 | J/molxK | 624.68 | Joback Method |
| cpg | 480.49 | J/molxK | 596.11 | Joback Method |
| cpg | 465.79 | J/molxK | 567.55 | Joback Method |
| cpg | 534.57 | J/molxK | 710.38 | Joback Method |
| dvisc | 0.0000753 | Paxs | 538.98 | Joback Method |
| dvisc | 0.0001052 | Paxs | 493.92 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001572 | Paxs | 448.86 | Joback Method |
| dvisc | 0.0002570 | Paxs | 403.80 | Joback Method |
| dvisc | 0.0004751 | Paxs | 358.73 | Joback Method |
| dvisc | 0.0010482 | Paxs | 313.67 | Joback Method |
| dvisc | 0.0030159 | Paxs | 268.61 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U332810&Units=SI |
| 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 |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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 |
| mvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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