

Pentaethylene glycol, monoethyl ether

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|-----------------------------|---|
| Other names: | 3,6,9,12,15-pentaoxaheptadecan-1-ol |
| Inchi: | InChI=1S/C12H26O6/c1-2-14-5-6-16-9-10-18-12-11-17-8-7-15-4-3-13/h13H,2-12H2,1H3 |
| InchiKey: | NJRFAMBTWHGSDE-UHFFFAOYSA-N |
| Formula: | C12H26O6 |
| SMILES: | CCOCCOCCOCCOCCOCCO |
| Mol. weight [g/mol]: | 266.33 |
| CAS: | 4353-29-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|---------|----------------|
| gf | -611.66 | kJ/mol | Joback Method |
| hf | -1104.34 | kJ/mol | Joback Method |
| hfus | 36.86 | kJ/mol | Joback Method |
| hvap | 71.04 | kJ/mol | Joback Method |
| log10ws | 0.45 | | Crippen Method |
| logp | 0.082 | | Crippen Method |
| mcvol | 215.160 | ml/mol | McGowan Method |
| pc | 1790.91 | kPa | Joback Method |
| rinpol | 1842.00 | | NIST Webbook |
| rinpol | 1842.00 | | NIST Webbook |
| tb | 678.24 | K | Joback Method |
| tc | 841.15 | K | Joback Method |
| tf | 396.97 | K | Joback Method |
| vc | 0.817 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 619.90 | J/molxK | 678.24 | Joback Method |
| cpg | 634.20 | J/molxK | 705.39 | Joback Method |
| cpg | 647.94 | J/molxK | 732.54 | Joback Method |
| cpg | 661.10 | J/molxK | 759.70 | Joback Method |
| cpg | 673.66 | J/molxK | 786.85 | Joback Method |
| cpg | 685.60 | J/molxK | 814.00 | Joback Method |

| | | | | |
|-------|-----------|---------|--------|---------------|
| cpg | 696.91 | J/molxK | 841.15 | Joback Method |
| dvisc | 0.0008989 | Paxs | 396.97 | Joback Method |
| dvisc | 0.0003297 | Paxs | 443.85 | Joback Method |
| dvisc | 0.0001464 | Paxs | 490.73 | Joback Method |
| dvisc | 0.0000749 | Paxs | 537.61 | Joback Method |
| dvisc | 0.0000427 | Paxs | 584.48 | Joback Method |
| dvisc | 0.0000264 | Paxs | 631.36 | Joback Method |
| dvisc | 0.0000175 | Paxs | 678.24 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C4353291&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307i |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| mcvol: | 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 |

Latest version available from:

<https://www.chemeo.com/cid/93-830-7/Pentaethylene-glycol-monoethyl-ether.pdf>

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