

14-Chloroheptadecanoic acid, methyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C18H35ClO2/c1-3-14-17(19)15-12-10-8-6-4-5-7-9-11-13-16-18(20)21-2/h17H, |
| InchiKey: | WGCAKLSPMJYGDF-UHFFFAOYSA-N |
| Formula: | C18H35ClO2 |
| SMILES: | CCCC(Cl)CCCCCCCCCCCCC(=O)OC |
| Mol. weight [g/mol]: | 318.92 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -147.61 | kJ/mol | Joback Method |
| hf | -680.67 | kJ/mol | Joback Method |
| hfus | 45.84 | kJ/mol | Joback Method |
| hvap | 68.81 | kJ/mol | Joback Method |
| log10ws | -6.48 | | Crippen Method |
| logp | 6.248 | | Crippen Method |
| mcvol | 284.160 | ml/mol | McGowan Method |
| pc | 1165.63 | kPa | Joback Method |
| ripol | 2226.00 | | NIST Webbook |
| ripol | 2214.00 | | NIST Webbook |
| ripol | 2692.00 | | NIST Webbook |
| ripol | 2675.00 | | NIST Webbook |
| ripol | 2692.00 | | NIST Webbook |
| tb | 724.52 | K | Joback Method |
| tc | 899.87 | K | Joback Method |
| tf | 379.70 | K | Joback Method |
| vc | 1.111 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 825.77 | J/molxK | 724.52 | Joback Method |
| cpg | 908.06 | J/molxK | 870.64 | Joback Method |
| cpg | 893.27 | J/molxK | 841.42 | Joback Method |
| cpg | 877.67 | J/molxK | 812.19 | Joback Method |
| cpg | 861.23 | J/molxK | 782.97 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 843.94 | J/mol×K | 753.74 | Joback Method |
| cpg | 922.05 | J/mol×K | 899.87 | Joback Method |
| dvisc | 0.0000780 | Paxs | 724.52 | Joback Method |
| dvisc | 0.0001060 | Paxs | 667.05 | Joback Method |
| dvisc | 0.0001527 | Paxs | 609.58 | Joback Method |
| dvisc | 0.0002373 | Paxs | 552.11 | Joback Method |
| dvisc | 0.0004087 | Paxs | 494.64 | Joback Method |
| dvisc | 0.0008119 | Paxs | 437.17 | Joback Method |
| dvisc | 0.0019853 | Paxs | 379.70 | 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=R308999&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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