

4-Chlorooctadecanoic acid, methyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C19H37ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18(20)16-17-19(21)22-2/h18 |
| InchiKey: | MUMYIMQHUCUCGL-UHFFFAOYSA-N |
| Formula: | C19H37ClO2 |
| SMILES: | CCCCCCCCCCCC(CI)CCC(=O)OC |
| Mol. weight [g/mol]: | 332.95 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -139.19 | kJ/mol | Joback Method |
| hf | -701.31 | kJ/mol | Joback Method |
| hfus | 48.43 | kJ/mol | Joback Method |
| hvap | 71.04 | kJ/mol | Joback Method |
| log10ws | -6.90 | | Crippen Method |
| logp | 6.638 | | Crippen Method |
| mcvol | 298.250 | ml/mol | McGowan Method |
| pc | 1092.82 | kPa | Joback Method |
| rinpola | 2291.00 | | NIST Webbook |
| ripola | 2724.00 | | NIST Webbook |
| tb | 747.40 | K | Joback Method |
| tc | 924.01 | K | Joback Method |
| tf | 390.97 | K | Joback Method |
| vc | 1.167 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 884.74 | J/molxK | 747.40 | Joback Method |
| cpg | 903.32 | J/molxK | 776.83 | Joback Method |
| cpg | 920.97 | J/molxK | 806.27 | Joback Method |
| cpg | 937.72 | J/molxK | 835.70 | Joback Method |
| cpg | 953.60 | J/molxK | 865.14 | Joback Method |
| cpg | 968.63 | J/molxK | 894.57 | Joback Method |
| cpg | 982.84 | J/molxK | 924.01 | Joback Method |
| dvisc | 0.0017764 | Paxs | 390.97 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0007200 | Paxs | 450.38 | Joback Method |
| dvisc | 0.0003602 | Paxs | 509.78 | Joback Method |
| dvisc | 0.0002082 | Paxs | 569.18 | Joback Method |
| dvisc | 0.0001335 | Paxs | 628.59 | Joback Method |
| dvisc | 0.0000924 | Paxs | 687.99 | Joback Method |
| dvisc | 0.0000678 | Paxs | 747.40 | 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=R309412&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/99-600-6/4-Chlorooctadecanoic-acid-methyl-ester.pdf>

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