# Hydratropic acid, heptyl ester

**Inchi:** InChI=1S/C16H24O2/c1-3-4-5-6-10-13-18-16(17)14(2)15-11-8-7-9-12-15/h7-9,11-12,14H
**InchiKey:** KFKOTBBAYXQTPD-UHFFFAOYSA-N
**Formula:** C16H24O2
**SMILES:** CCCCCCCOC(=O)C(C)c1ccccc1
**Mol. weight [g/mol]:** 248.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -40.11 | kJ/mol | Joback Method |
| hf | -387.12 | kJ/mol | Joback Method |
| hfus | 30.50 | kJ/mol | Joback Method |
| hvap | 62.25 | kJ/mol | Joback Method |
| log10ws | -4.45 | | Crippen Method |
| logp | 4.304 | | Crippen Method |
| mcvol | 219.980 | ml/mol | McGowan Method |
| pc | 1781.84 | kPa | Joback Method |
| rinpol | 2279.00 | | NIST Webbook |
| rinpol | 2279.00 | | NIST Webbook |
| tb | 668.01 | K | Joback Method |
| tc | 866.60 | K | Joback Method |
| tf | 353.66 | K | Joback Method |
| vc | 0.842 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 600.45 | J/mol×K | 668.01 | Joback Method |
| cpg | 617.94 | J/mol×K | 701.11 | Joback Method |
| cpg | 634.43 | J/mol×K | 734.21 | Joback Method |
| cpg | 649.95 | J/mol×K | 767.31 | Joback Method |
| cpg | 664.53 | J/mol×K | 800.40 | Joback Method |
| cpg | 678.21 | J/mol×K | 833.50 | Joback Method |
| cpg | 691.01 | J/mol×K | 866.60 | Joback Method |
| dvisc | 0.0022754 | Pa×s | 353.66 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0009989 | Pa×s | 406.05 | Joback Method |
| dvisc | 0.0005293 | Pa×s | 458.44 | Joback Method |
| dvisc | 0.0003195 | Pa×s | 510.84 | Joback Method |
| dvisc | 0.0002118 | Pa×s | 563.23 | Joback Method |
| dvisc | 0.0001506 | Pa×s | 615.62 | Joback Method |
| dvisc | 0.0001130 | Pa×s | 668.01 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=U415064&Units=SI |

# 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 |