

Adipic acid, hexyl 3-methylbutyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C17H32O4/c1-4-5-6-9-13-20-16(18)10-7-8-11-17(19)21-14-12-15(2)3/h15H,4- |
| InchiKey: | PKUSJQIUSYROMX-UHFFFAOYSA-N |
| Formula: | C17H32O4 |
| SMILES: | CCCCCOC(=O)CCCC(=O)OCCC(C)C |
| Mol. weight [g/mol]: | 300.43 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -378.02 | kJ/mol | Joback Method |
| hf | -889.09 | kJ/mol | Joback Method |
| hfus | 41.84 | kJ/mol | Joback Method |
| hvap | 71.36 | kJ/mol | Joback Method |
| log10ws | -4.42 | | Crippen Method |
| logp | 4.260 | | Crippen Method |
| mvol | 265.270 | ml/mol | McGowan Method |
| pc | 1322.31 | kPa | Joback Method |
| rinpol | 2014.00 | | NIST Webbook |
| rinpol | 2014.00 | | NIST Webbook |
| tb | 740.50 | K | Joback Method |
| tc | 919.30 | K | Joback Method |
| tf | 410.67 | K | Joback Method |
| vc | 1.030 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 791.52 | J/molxK | 740.50 | Joback Method |
| cpg | 808.68 | J/molxK | 770.30 | Joback Method |
| cpg | 824.95 | J/molxK | 800.10 | Joback Method |
| cpg | 840.35 | J/molxK | 829.90 | Joback Method |
| cpg | 854.88 | J/molxK | 859.70 | Joback Method |
| cpg | 868.56 | J/molxK | 889.50 | Joback Method |
| cpg | 881.39 | J/molxK | 919.30 | Joback Method |
| dvisc | 0.0013763 | Paxs | 410.67 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0006360 | Paxs | 465.64 | Joback Method |
| dvisc | 0.0003459 | Paxs | 520.61 | Joback Method |
| dvisc | 0.0002113 | Paxs | 575.59 | Joback Method |
| dvisc | 0.0001407 | Paxs | 630.56 | Joback Method |
| dvisc | 0.0001000 | Paxs | 685.53 | Joback Method |
| dvisc | 0.0000748 | Paxs | 740.50 | 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=U348968&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

Legend

| | |
|---------------------------------------|---|
| cp_g: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| g_f: | Standard Gibbs free energy of formation |
| h_f: | Enthalpy of formation at standard conditions |
| h_{fus}: | Enthalpy of fusion at standard conditions |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀w_s: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rin_{pol}: | Non-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/56-392-5/Adipic-acid-hexyl-3-methylbutyl-ester.pdf>

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