

Adipic acid, 3-hexyl isobutyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C16H30O4/c1-5-9-14(6-2)20-16(18)11-8-7-10-15(17)19-12-13(3)4/h13-14H,5-

ZUKDAKMLEHKWPL-UHFFFAOYSA-N

C16H30O4

CCCC(CC)OC(=O)CCCCC(=O)OCC(C)C

286.41

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -388.88 | kJ/mol | Joback Method |
| hf | -873.73 | kJ/mol | Joback Method |
| hfus | 35.72 | kJ/mol | Joback Method |
| hvap | 68.75 | kJ/mol | Joback Method |
| log10ws | -4.12 | | Crippen Method |
| logp | 3.868 | | Crippen Method |
| mcvol | 251.180 | ml/mol | McGowan Method |
| pc | 1428.30 | kPa | Joback Method |
| rinpol | 1822.00 | | NIST Webbook |
| rinpol | 1822.00 | | NIST Webbook |
| tb | 717.18 | K | Joback Method |
| tc | 897.32 | K | Joback Method |
| tf | 384.40 | K | Joback Method |
| vc | 0.968 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 734.56 | J/molxK | 717.18 | Joback Method |
| cpg | 751.53 | J/molxK | 747.20 | Joback Method |
| cpg | 767.64 | J/molxK | 777.23 | Joback Method |
| cpg | 782.89 | J/molxK | 807.25 | Joback Method |
| cpg | 797.29 | J/molxK | 837.27 | Joback Method |
| cpg | 810.84 | J/molxK | 867.29 | Joback Method |
| cpg | 823.57 | J/molxK | 897.32 | Joback Method |
| dvisc | 0.0018907 | Paxs | 384.40 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0007981 | Paxs | 439.86 | Joback Method |
| dvisc | 0.0004087 | Paxs | 495.33 | Joback Method |
| dvisc | 0.0002395 | Paxs | 550.79 | Joback Method |
| dvisc | 0.0001547 | Paxs | 606.25 | Joback Method |
| dvisc | 0.0001076 | Paxs | 661.72 | Joback Method |
| dvisc | 0.0000791 | Paxs | 717.18 | 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=U353622&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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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