

Adipic acid, ethyl 3-methylbutyl ester

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|----------------------|--------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C13H24O4/c1-4-16-12(14)7-5-6-8-13(15)17-10-9-11(2)3/h11H,4-10H2,1-3H3 |
| InchiKey: | KFGVPPDQMGNYPH-UHFFFAOYSA-N |
| Formula: | C13H24O4 |
| SMILES: | CCOC(=O)CCCCC(=O)OCCC(C)C |
| Mol. weight [g/mol]: | 244.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -411.70 | kJ/mol | Joback Method |
| hf | -806.53 | kJ/mol | Joback Method |
| hfus | 31.48 | kJ/mol | Joback Method |
| hvap | 62.46 | kJ/mol | Joback Method |
| log10ws | -2.75 | | Crippen Method |
| logp | 2.699 | | Crippen Method |
| mcvol | 208.910 | ml/mol | McGowan Method |
| pc | 1786.37 | kPa | Joback Method |
| rinpol | 1621.00 | | NIST Webbook |
| tb | 648.98 | K | Joback Method |
| tc | 828.08 | K | Joback Method |
| tf | 365.59 | K | Joback Method |
| vc | 0.805 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 568.82 | J/molxK | 648.98 | Joback Method |
| cpg | 584.20 | J/molxK | 678.83 | Joback Method |
| cpg | 598.88 | J/molxK | 708.68 | Joback Method |
| cpg | 612.86 | J/molxK | 738.53 | Joback Method |
| cpg | 626.13 | J/molxK | 768.38 | Joback Method |
| cpg | 638.71 | J/molxK | 798.23 | Joback Method |
| cpg | 650.59 | J/molxK | 828.08 | Joback Method |
| dvisc | 0.0019834 | Paxs | 365.59 | Joback Method |
| dvisc | 0.0009630 | Paxs | 412.82 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0005423 | Paxs | 460.05 | Joback Method |
| dvisc | 0.0003399 | Paxs | 507.29 | Joback Method |
| dvisc | 0.0002306 | Paxs | 554.52 | Joback Method |
| dvisc | 0.0001663 | Paxs | 601.75 | Joback Method |
| dvisc | 0.0001258 | Paxs | 648.98 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U347862&Units=SI |
| 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 |

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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