

Butanoic acid, 2-octyl ester

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|-----------------------------|---|
| Other names: | 1-Methylheptyl butyrate Butanoic acid, 1-methylheptyl ester |
| Inchi: | InChI=1S/C12H24O2/c1-4-6-7-8-10-11(3)14-12(13)9-5-2/h11H,4-10H2,1-3H3 |
| InchiKey: | RBIWXCXZWBFGAA-UHFFFAOYSA-N |
| Formula: | C12H24O2 |
| SMILES: | CCCCCCC(C)OC(=O)CCC |
| Mol. weight [g/mol]: | 200.32 |
| CAS: | 20286-44-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|----------------------|----------------|
| gf | -186.20 | kJ/mol | Joback Method |
| hf | -541.09 | kJ/mol | Joback Method |
| hfus | 26.10 | kJ/mol | Joback Method |
| hvap | 51.07 | kJ/mol | Joback Method |
| log10ws | -3.82 | | Crippen Method |
| logp | 3.689 | | Crippen Method |
| mcvol | 187.380 | ml/mol | McGowan Method |
| pc | 1864.33 | kPa | Joback Method |
| rinpol | 1298.00 | | NIST Webbook |
| rinpol | 1298.00 | | NIST Webbook |
| ripol | 1507.00 | | NIST Webbook |
| tb | 492.00 ± 5.00 | K | NIST Webbook |
| tc | 722.69 | K | Joback Method |
| tf | 282.16 | K | Joback Method |
| vc | 0.726 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 464.44 | J/mol×K | 549.81 | Joback Method |
| cpg | 480.46 | J/mol×K | 578.62 | Joback Method |
| cpg | 495.83 | J/mol×K | 607.44 | Joback Method |
| cpg | 510.57 | J/mol×K | 636.25 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 524.69 | J/molxK | 665.07 | Joback Method |
| cpg | 538.20 | J/molxK | 693.88 | Joback Method |
| cpg | 551.11 | J/molxK | 722.69 | Joback Method |
| dvisc | 0.0042661 | Paxs | 282.16 | Joback Method |
| dvisc | 0.0017460 | Paxs | 326.77 | Joback Method |
| dvisc | 0.0008857 | Paxs | 371.38 | Joback Method |
| dvisc | 0.0005197 | Paxs | 415.99 | Joback Method |
| dvisc | 0.0003381 | Paxs | 460.59 | Joback Method |
| dvisc | 0.0002373 | Paxs | 505.20 | Joback Method |
| dvisc | 0.0001764 | Paxs | 549.81 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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=C20286446&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 |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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