

2-Butoxy-1-propanol

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|-----------------------------|---|
| Other names: | Butoxypropanol 2-Butoxypropanol butoxypropan-1-ol |
| Inchi: | InChI=1S/C7H16O2/c1-3-4-5-9-7(2)6-8/h7-8H,3-6H2,1-2H3 |
| InchiKey: | WGKZYJXRTIPTCV-UHFFFAOYSA-N |
| Formula: | C7H16O2 |
| SMILES: | CCCCOC(C)CO |
| Mol. weight [g/mol]: | 132.20 |
| CAS: | 29387-86-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -236.20 | kJ/mol | Joback Method |
| hf | -477.54 | kJ/mol | Joback Method |
| hfus | 15.64 | kJ/mol | Joback Method |
| hvap | 49.88 | kJ/mol | Joback Method |
| log10ws | -1.22 | | Crippen Method |
| logp | 1.184 | | Crippen Method |
| mcvol | 121.230 | ml/mol | McGowan Method |
| pc | 3062.55 | kPa | Joback Method |
| rinpol | 934.00 | | NIST Webbook |
| rinpol | 934.00 | | NIST Webbook |
| rinpol | 951.00 | | NIST Webbook |
| rinpol | 951.00 | | NIST Webbook |
| ripol | 1350.00 | | NIST Webbook |
| ripol | 1422.20 | | NIST Webbook |
| ripol | 1350.00 | | NIST Webbook |
| tb | 473.72 | K | Joback Method |
| tc | 637.45 | K | Joback Method |
| tf | 236.70 | K | Joback Method |
| vc | 0.459 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 271.52 | J/mol×K | 473.72 | Joback Method |
| cpg | 321.47 | J/mol×K | 610.16 | Joback Method |
| cpg | 312.18 | J/mol×K | 582.87 | Joback Method |
| cpg | 302.54 | J/mol×K | 555.59 | Joback Method |
| cpg | 292.56 | J/mol×K | 528.30 | Joback Method |
| cpg | 282.22 | J/mol×K | 501.01 | Joback Method |
| cpg | 330.41 | J/mol×K | 637.45 | Joback Method |
| dvisc | 0.0001517 | Paxs | 473.72 | Joback Method |
| dvisc | 0.0002622 | Paxs | 434.22 | Joback Method |
| dvisc | 0.0005057 | Paxs | 394.71 | Joback Method |
| dvisc | 0.0011285 | Paxs | 355.21 | Joback Method |
| dvisc | 0.0030786 | Paxs | 315.71 | Joback Method |
| dvisc | 0.0111917 | Paxs | 276.20 | Joback Method |
| dvisc | 0.0625947 | Paxs | 236.70 | 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=C29387868&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpolar: | Non-polar retention indices |
| ripolar: | Polar retention indices |

tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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