

Isobutyl

(1-((1-methoxypropan-2-yl)oxy)propan-2-yl)

InChI: InChI=1S/C12H24O5/c1-9(2)6-16-12(13)17-11(4)8-15-10(3)7-14-5/h9-11H,6-8H2,1-5H3
carbonate

InChIKey: JZARTOGQMAIVPJ-UHFFFAOYSA-N

Formula: C12H24O5

SMILES: COCC(C)OCC(C)OC(=O)OCC(C)C

Mol. weight [g/mol]: 248.32

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -506.08 | kJ/mol | Joback Method |
| hf | -948.31 | kJ/mol | Joback Method |
| hfus | 22.62 | kJ/mol | Joback Method |
| hvap | 57.53 | kJ/mol | Joback Method |
| log10ws | -1.93 | | Crippen Method |
| logp | 2.236 | | Crippen Method |
| mcvol | 204.990 | ml/mol | McGowan Method |
| pc | 1809.23 | kPa | Joback Method |
| rinpol | 1466.00 | | NIST Webbook |
| tb | 616.19 | K | Joback Method |
| tc | 793.60 | K | Joback Method |
| tf | 318.85 | K | Joback Method |
| vc | 0.767 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 549.28 | J/molxK | 616.19 | Joback Method |
| cpg | 622.80 | J/molxK | 764.03 | Joback Method |
| cpg | 609.44 | J/molxK | 734.47 | Joback Method |
| cpg | 595.39 | J/molxK | 704.90 | Joback Method |
| cpg | 580.67 | J/molxK | 675.33 | Joback Method |
| cpg | 565.30 | J/molxK | 645.76 | Joback Method |
| cpg | 635.46 | J/molxK | 793.60 | Joback Method |
| dvisc | 0.0000750 | Paxs | 616.19 | Joback Method |
| dvisc | 0.0001037 | Paxs | 566.63 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001528 | Paxs | 517.08 | Joback Method |
| dvisc | 0.0002442 | Paxs | 467.52 | Joback Method |
| dvisc | 0.0004363 | Paxs | 417.96 | Joback Method |
| dvisc | 0.0009112 | Paxs | 368.41 | Joback Method |
| dvisc | 0.0023927 | Paxs | 318.85 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U378288&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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