

Isopropyl [2-chloro-1-(chloromethyl)ethyl] ether

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|----------------------|---|
| Inchi: | InChI=1S/C6H12Cl2O/c1-5(2)9-6(3,8)4-7/h5H,4H2,1-3H3 |
| InchiKey: | VKTMECFEGQKZCB-UHFFFAOYSA-N |
| Formula: | C6H12Cl2O |
| SMILES: | CC(C)OC(C)(Cl)CCl |
| Mol. weight [g/mol]: | 171.06 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -128.82 | kJ/mol | Joback Method |
| hf | -344.90 | kJ/mol | Joback Method |
| hfus | 9.94 | kJ/mol | Joback Method |
| hvap | 38.45 | kJ/mol | Joback Method |
| log10ws | -2.45 | | Crippen Method |
| logp | 2.605 | | Crippen Method |
| mcvol | 125.750 | ml/mol | McGowan Method |
| pc | 2896.73 | kPa | Joback Method |
| tb | 430.29 | K | Joback Method |
| tc | 626.41 | K | Joback Method |
| tf | 226.87 | K | Joback Method |
| vc | 0.470 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 236.94 | J/molxK | 430.29 | Joback Method |
| cpg | 248.34 | J/molxK | 462.98 | Joback Method |
| cpg | 259.15 | J/molxK | 495.66 | Joback Method |
| cpg | 269.39 | J/molxK | 528.35 | Joback Method |
| cpg | 279.08 | J/molxK | 561.03 | Joback Method |
| cpg | 288.25 | J/molxK | 593.72 | Joback Method |
| cpg | 296.90 | J/molxK | 626.41 | Joback Method |
| dvisc | 0.0082137 | Paxs | 226.87 | Joback Method |
| dvisc | 0.0032489 | Paxs | 260.77 | Joback Method |
| dvisc | 0.0015908 | Paxs | 294.68 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0009026 | Paxs | 328.58 | Joback Method |
| dvisc | 0.0005694 | Paxs | 362.48 | Joback Method |
| dvisc | 0.0003886 | Paxs | 396.39 | Joback Method |
| dvisc | 0.0002817 | Paxs | 430.29 | 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=R629266&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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