

Alpha-chloropropionic acid anhydride

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|-----------------------------|---|
| Inchi: | InChI=1S/C6H8Cl2O3/c1-3(7)5(9)11-6(10)4(2)8/h3-4H,1-2H3 |
| InchiKey: | OAVBKHDCXXETQR-UHFFFAOYSA-N |
| Formula: | C6H8Cl2O3 |
| SMILES: | CC(Cl)C(=O)OC(=O)C(C)Cl |
| Mol. weight [g/mol]: | 199.03 |
| CAS: | 39060-20-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -391.94 | kJ/mol | Joback Method |
| hf | -566.59 | kJ/mol | Joback Method |
| hfus | 17.03 | kJ/mol | Joback Method |
| hvap | 52.85 | kJ/mol | Joback Method |
| log10ws | -1.50 | | Crippen Method |
| logp | 1.311 | | Crippen Method |
| mcvol | 128.890 | ml/mol | McGowan Method |
| pc | 3291.59 | kPa | Joback Method |
| tb | 540.82 | K | Joback Method |
| tc | 748.93 | K | Joback Method |
| tf | 309.31 | K | Joback Method |
| vc | 0.487 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 261.46 | J/molxK | 540.82 | Joback Method |
| cpg | 301.77 | J/molxK | 714.24 | Joback Method |
| cpg | 294.63 | J/molxK | 679.56 | Joback Method |
| cpg | 287.04 | J/molxK | 644.87 | Joback Method |
| cpg | 278.98 | J/molxK | 610.19 | Joback Method |
| cpg | 270.45 | J/molxK | 575.50 | Joback Method |
| cpg | 308.44 | J/molxK | 748.93 | Joback Method |
| dvisc | 0.0002864 | Paxs | 540.82 | Joback Method |
| dvisc | 0.0003755 | Paxs | 502.23 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0005152 | Paxs | 463.65 | Joback Method |
| dvisc | 0.0007485 | Paxs | 425.06 | Joback Method |
| dvisc | 0.0011717 | Paxs | 386.48 | Joback Method |
| dvisc | 0.0020260 | Paxs | 347.89 | Joback Method |
| dvisc | 0.0040160 | Paxs | 309.31 | 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=C39060203&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 |
| 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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