

Methacryloyl chloride

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| Other names: | 2-Methyl-2-propenoyl chloride 2-Methylpropenoic acid chloride 2-Methylpropenoyl chloride 2-Propenoyl chloride, 2-methyl- Methacryl chloride Methacrylic acid chloride Methacrylic chloride Methacrylyl chloride Methylacryloyl chloride «alpha»-Methylacryloyl chloride Â«alphaÂ»-Methylacryloyl chloride |
| Inchi: | InChI=1S/C4H5ClO/c1-3(2)4(5)6/h1H2,2H3 |
| InchiKey: | VHRYZQNGTZDNX-UHFFFAOYSA-N |
| Formula: | C4H5ClO |
| SMILES: | C=C(C)C(=O)Cl |
| Mol. weight [g/mol]: | 104.53 |
| CAS: | 920-46-7 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -78.76 | kJ/mol | Joback Method |
| hf | -138.57 | kJ/mol | Joback Method |
| hfus | 9.32 | kJ/mol | Joback Method |
| hvap | 35.04 | kJ/mol | Joback Method |
| log10ws | -1.28 | | Crippen Method |
| logp | 1.328 | | Crippen Method |
| mcvol | 76.730 | ml/mol | McGowan Method |
| pc | 4277.45 | kPa | Joback Method |
| tb | 369.20 | K | NIST Webbook |
| tc | 574.54 | K | Joback Method |
| tf | 198.97 | K | Joback Method |
| vc | 0.296 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 117.91 | J/mol×K | 378.78 | Joback Method |
| cpg | 124.25 | J/mol×K | 411.41 | Joback Method |
| cpg | 130.26 | J/mol×K | 444.03 | Joback Method |
| cpg | 135.96 | J/mol×K | 476.66 | Joback Method |
| cpg | 141.36 | J/mol×K | 509.29 | Joback Method |
| cpg | 146.47 | J/mol×K | 541.91 | Joback Method |
| cpg | 151.30 | J/mol×K | 574.54 | Joback Method |
| hvapt | 36.10 | kJ/mol | 342.50 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.25934e+01 |
| Coeff. B | -2.61866e+03 |
| Coeff. C | -5.85250e+01 |
| Temperature range (K), min. | 271.32 |
| Temperature range (K), max. | 418.14 |

Sources

| | |
|--------------------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C920467&Units=SI |
| The Yaws Handbook of Vapor Pressure: | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| 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 |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| pvap: | Vapor pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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