

# 2-Chloropropionamide

<b>Other names:</b>	Propanamide, 2-chloro-
<b>Inchi:</b>	InChI=1S/C3H6ClNO/c1-2(4)3(5)6/h2H,1H3,(H2,5,6)
<b>InchiKey:</b>	OEZPDHRXGCLGKB-UHFFFAOYSA-N
<b>Formula:</b>	C3H6ClNO
<b>SMILES:</b>	CC(Cl)C(N)=O
<b>Mol. weight [g/mol]:</b>	107.54
<b>CAS:</b>	27816-36-0

## Physical Properties

Property code	Value	Unit	Source
gf	-102.46	kJ/mol	Joback Method
hf	-205.06	kJ/mol	Joback Method
hfus	11.00	kJ/mol	Joback Method
hvap	43.66	kJ/mol	Joback Method
log10ws	-0.55		Crippen Method
logp	0.099		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
tb	431.43	K	Joback Method
tc	641.04	K	Joback Method
tf	271.68	K	Joback Method
vc	0.281	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.80	J/mol×K	431.43	Joback Method
cpg	144.37	J/mol×K	466.37	Joback Method
cpg	150.60	J/mol×K	501.30	Joback Method
cpg	156.50	J/mol×K	536.24	Joback Method
cpg	162.08	J/mol×K	571.17	Joback Method
cpg	167.35	J/mol×K	606.11	Joback Method
cpg	172.32	J/mol×K	641.04	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C27816360&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27816360&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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