3-Chloropropionamide

Other names: Propanamide, 3-chloro-
Inchi: InChI=1S/C3H6ClNO/c4-2-1-3(5)6/h1-2H2,(H2,5,6)
InchiKey: JQDXZJYAUSVHDH-UHFFFAOYSA-N
Formula: C3H6ClNO
SMILES: NC(=O)CCCl
Mol. weight [g/mol]: 107.54
CAS: 5875-24-1

Physical Properties

Property code	Value	Unit	Source
gf	-100.02	kJ/mol	Joback Method
hf	-199.78	kJ/mol	Joback Method
hfus	14.52	kJ/mol	Joback Method
hvap	44.04	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.101		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	4938.44	kPa	Joback Method
tb	431.87	K	Joback Method
tc	636.51	K	Joback Method
tf	286.68	K	Joback Method
vc	0.287	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.65	J/mol×K	431.87	Joback Method
cpg	143.97	J/mol×K	465.98	Joback Method
cpg	149.97	J/mol×K	500.08	Joback Method
cpg	155.67	J/mol×K	534.19	Joback Method
cpg	161.08	J/mol×K	568.30	Joback Method
cpg	166.19	J/mol×K	602.40	Joback Method
cpg	171.03	J/mol×K	636.51	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5875241&Units=SI

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
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