Propanamide, 3-chloro-2,2-dimethyl-

Inchi: InChI=1S/C5H10ClNO/c1-5(2,3-6)4(7)8/h3H2,1-2H3,(H2,7,8)
InchiKey: CCFNEVMWSYAQKL-UHFFFAOYSA-N
Formula: C5H10ClNO
SMILES: CC(C)(CCl)C(N)=O
Mol. weight [g/mol]: 135.59
CAS: 41461-75-0

Physical Properties

Property code	Value	Unit	Source
gf	-80.34	kJ/mol	Joback Method
hf	-249.81	kJ/mol	Joback Method
hfus	12.29	kJ/mol	Joback Method
hvap	47.20	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.737		Crippen Method
mcvol	105.100	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	474.40	K	Joback Method
tc	687.40	K	Joback Method
tf	382.00 ± 3.00	K	NIST Webbook
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.09	J/mol×K	474.40	Joback Method
cpg	226.13	J/mol×K	509.90	Joback Method
cpg	235.51	J/mol×K	545.40	Joback Method
cpg	244.25	J/mol×K	580.90	Joback Method
cpg	252.40	J/mol×K	616.40	Joback Method
cpg	259.99	J/mol×K	651.90	Joback Method
cpg	267.05	J/mol×K	687.40	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=C41461750&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