Chloroacetamide, N-ethyl-N-isobutyl-

Inchi: InChI=1S/C8H16ClNO/c1-4-10(6-7(2)3)8(11)5-9/h7H,4-6H2,1-3H3
InchiKey: NFYZIEFIGBHLBZ-UHFFFAOYSA-N
Formula: C8H16ClNO
SMILES: CCN(CC(C)C)C(=O)CCl
Mol. weight [g/mol]: 177.67

Physical Properties

Property code	Value	Unit	Source
gf	-16.03	kJ/mol	Joback Method
hf	-274.52	kJ/mol	Joback Method
hfus	21.77	kJ/mol	Joback Method
hvap	46.19	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.730		Crippen Method
mcvol	147.370	ml/mol	McGowan Method
pc	2619.09	kPa	Joback Method
rinpol	1351.00		NIST Webbook
rinpol	1351.00		NIST Webbook
tb	485.74	K	Joback Method
tc	669.26	K	Joback Method
tf	277.24	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.34	J/mol×K	485.74	Joback Method
cpg	329.60	J/mol×K	516.33	Joback Method
cpg	342.22	J/mol×K	546.91	Joback Method
cpg	354.23	J/mol×K	577.50	Joback Method
cpg	365.63	J/mol×K	608.09	Joback Method
cpg	376.46	J/mol×K	638.68	Joback Method
cpg	386.73	J/mol×K	669.26	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=U415264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume