Chloroacetamide, N-ethyl-N-propyl-

Inchi: InChI=1S/C7H14ClNO/c1-3-5-9(4-2)7(10)6-8/h3-6H2,1-2H3
InchiKey: QYCUBRKBUVRFKJ-UHFFFAOYSA-N
Formula: C7H14ClNO
SMILES: CCCN(CC)C(=O)CCl
Mol. weight [g/mol]: 163.65

Physical Properties

Property code	Value	Unit	Source
gf	-22.01	kJ/mol	Joback Method
hf	-248.60	kJ/mol	Joback Method
hfus	22.70	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.484		Crippen Method
mcvol	133.280	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	463.30	K	Joback Method
tc	644.68	K	Joback Method
tf	280.97	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.26	J/mol×K	463.30	Joback Method
cpg	285.23	J/mol×K	493.53	Joback Method
cpg	296.62	J/mol×K	523.76	Joback Method
cpg	307.48	J/mol×K	553.99	Joback Method
cpg	317.80	J/mol×K	584.22	Joback Method
cpg	327.61	J/mol×K	614.45	Joback Method
cpg	336.93	J/mol×K	644.68	Joback Method

Sources

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=U415263&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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