Chloroacetamide, N-ethyl-N-pentyl-

Inchi: InChI=1S/C9H18ClNO/c1-3-5-6-7-11(4-2)9(12)8-10/h3-8H2,1-2H3
InchiKey: YGNJFQDHCDYXNA-UHFFFAOYSA-N
Formula: C9H18ClNO
SMILES: CCCCCN(CC)C(=O)CCl
Mol. weight [g/mol]: 191.70

Physical Properties

Property code	Value	Unit	Source
gf	-5.17	kJ/mol	Joback Method
hf	-289.88	kJ/mol	Joback Method
hfus	27.88	kJ/mol	Joback Method
hvap	48.80	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	2.264		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	509.06	K	Joback Method
tc	687.08	K	Joback Method
tf	303.51	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.00	J/mol×K	509.06	Joback Method
cpg	374.75	J/mol×K	538.73	Joback Method
cpg	387.86	J/mol×K	568.40	Joback Method
cpg	400.35	J/mol×K	598.07	Joback Method
cpg	412.23	J/mol×K	627.74	Joback Method
cpg	423.54	J/mol×K	657.41	Joback Method
cpg	434.29	J/mol×K	687.08	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=U415267&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

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