

Chloroacetamide, N-ethyl-N-hexyl-

Inchi:	InChI=1S/C10H20ClNO/c1-3-5-6-7-8-12(4-2)10(13)9-11/h3-9H2,1-2H3
InchiKey:	CJVHBUUCGKGZYBI-UHFFFAOYSA-N
Formula:	C10H20ClNO
SMILES:	CCCCCCN(CC)C(=O)CCl
Mol. weight [g/mol]:	205.72

Physical Properties

Property code	Value	Unit	Source
gf	3.25	kJ/mol	Joback Method
hf	-310.52	kJ/mol	Joback Method
hfus	30.47	kJ/mol	Joback Method
hvap	51.03	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.654		Crippen Method
mcvol	175.550	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	1875.00		NIST Webbook
tb	531.94	K	Joback Method
tc	708.34	K	Joback Method
tf	314.78	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.68	J/mol×K	531.94	Joback Method
cpg	422.18	J/mol×K	561.34	Joback Method
cpg	436.00	J/mol×K	590.74	Joback Method
cpg	449.17	J/mol×K	620.14	Joback Method
cpg	461.71	J/mol×K	649.54	Joback Method
cpg	473.64	J/mol×K	678.94	Joback Method
cpg	484.98	J/mol×K	708.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415268&Units=SI
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

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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