

Chloroacetamide, N-ethyl-N-3-methylbutyl-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C9H18ClNO/c1-4-11(9(12)7-10)6-5-8(2)3/h8H,4-7H2,1-3H3

JQTOQUGGWYCWII-UHFFFAOYSA-N

C9H18ClNO

CCN(CCC(C)C)C(=O)CCl

191.70

Physical Properties

Property code	Value	Unit	Source
gf	-7.61	kJ/mol	Joback Method
hf	-295.16	kJ/mol	Joback Method
hfus	24.36	kJ/mol	Joback Method
hvap	48.41	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	2.120		Crippen Method
mcvol	161.460	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinpol	1487.00		NIST Webbook
rinpol	1487.00		NIST Webbook
tb	508.62	K	Joback Method
tc	690.28	K	Joback Method
tf	288.51	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.23	J/mol×K	508.62	Joback Method
cpg	375.33	J/mol×K	538.90	Joback Method
cpg	388.75	J/mol×K	569.17	Joback Method
cpg	401.52	J/mol×K	599.45	Joback Method
cpg	413.66	J/mol×K	629.73	Joback Method
cpg	425.19	J/mol×K	660.00	Joback Method
cpg	436.13	J/mol×K	690.28	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=U415266&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	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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