

N-(2-Chloroethyl)acetamide

Other names:	Acetamide, N-(2-chloroethyl)-
Inchi:	InChI=1S/C4H8ClNO/c1-4(7)6-3-2-5/h2-3H2,1H3,(H,6,7)
InchiKey:	HSKNJSHFPPHTAQ-UHFFFAOYSA-N
Formula:	C4H8ClNO
SMILES:	CC(O)=NCCCl
Mol. weight [g/mol]:	121.56
CAS:	7355-58-0

Physical Properties

Property code	Value	Unit	Source
hf	-221.43	kJ/mol	Joback Method
hvap	48.96	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	1.202		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
tb	497.09	K	Joback Method
tc	689.02	K	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.50 ± 1.50	K	2.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7355580&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

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