Acetamide, 2-chloro-

Other names:	2-Chloroacetamide
	2-Chloroethanamide
	Acetamide, «alpha»-chloro-
	Acetamide, Â«alphaÂ»-chloro-
	Chloracetamid
	Chloracetamide
	Chloroacetamide
	Mergal AF
	Microcide
	NSC 54286
	USAF DO-29
	alpha-Chloroacetamide
	«alpha»-Chloracetamide
	«alpha»-Chloroacetamide
	Â«alphaÂ»-Chloracetamide
	Â«alphaÂ»-Chloroacetamide
Inchi:	InChI=1S/C2H4ClNO/c3-1-2(4)5/h1H2,(H2,4,5)
InchiKey:	VXIVSQZSERGHQP-UHFFFAOYSA-N
Formula:	C2H4ClNO
SMILES:	NC(=O)CCl
Mol. weight [g/mol]:	93.51
CAS:	79-07-2

Physical Properties

Property code	Value	Unit	Source
chs	-1041.00	kJ/mol	NIST Webbook
chs	-1044.00 ± 8.40	kJ/mol	NIST Webbook
gf	-108.44	kJ/mol	Joback Method
hf	-179.14	kJ/mol	Joback Method
hfs	-338.00 ± 8.40	kJ/mol	NIST Webbook
hfus	11.93	kJ/mol	Joback Method
hvap	41.82	kJ/mol	Joback Method
log10ws	-0.02		Aqueous Solubility Prediction Method
log10ws	-0.02		Estimated Solubility Method
logp	-0.289		Crippen Method

mcvol	62.830	ml/mol	McGowan Method
pc	5678.82	kPa	Joback Method
tb	408.99	K	Joback Method
tc	615.87	K	Joback Method
tf	392.65	K	Aqueous Solubility Prediction Method
vc	0.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.57	J/mol×K	408.99	Joback Method
cpg	108.27	J/mol×K	443.47	Joback Method
cpg	112.74	J/mol×K	477.95	Joback Method
cpg	116.98	J/mol×K	512.43	Joback Method
cpg	121.00	J/mol×K	546.91	Joback Method
cpg	124.80	J/mol×K	581.39	Joback Method
cpg	128.39	J/mol×K	615.87	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79072&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume