

Carbamic acid, 2-chloroethyl ester

Other names:	Ethanol, 2-chloro-, carbamate «beta»-Chloroethyl carbamate Chloroethyl carbamate 2-Chloroethyl carbamate Carbamic acid, «beta»-chloroethyl ester
Inchi:	InChI=1S/C3H6ClNO2/c4-1-2-7-3(5)6/h1-2H2,(H2,5,6)
InchiKey:	LIJLYNWYKULUHA-UHFFFAOYSA-N
Formula:	C3H6ClNO2
SMILES:	NC(=O)OCCCl
Mol. weight [g/mol]:	123.54
CAS:	2114-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-205.02	kJ/mol	Joback Method
hf	-332.00	kJ/mol	Joback Method
hfus	15.71	kJ/mol	Joback Method
hvap	46.45	kJ/mol	Joback Method
log10ws	-0.51		Crippen Method
logp	0.321		Crippen Method
mcvol	82.790	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
tb	454.29	K	Joback Method
tc	657.71	K	Joback Method
tf	308.91	K	Joback Method
vc	0.305	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	156.40	J/mol×K	454.29	Joback Method
cpg	162.64	J/mol×K	488.19	Joback Method
cpg	168.65	J/mol×K	522.10	Joback Method
cpg	174.42	J/mol×K	556.00	Joback Method

cpg	179.95	J/mol×K	589.91	Joback Method
cpg	185.23	J/mol×K	623.81	Joback Method
cpg	190.25	J/mol×K	657.71	Joback Method

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=C2114183&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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