N,N-Dichlorourethan

Other names: Carbamic acid, dichloro-, ethyl ester
Inchi: InChI=1S/C3H5Cl2NO2/c1-2-8-3(7)6(4)5/h2H2,1H3
InchiKey: PCGGNOFZZFFFLU-UHFFFAOYSA-N
Formula: C3H5Cl2NO2
SMILES: CCOC(=O)N(Cl)Cl
Mol. weight [g/mol]: 157.98
CAS: 13698-16-3

Physical Properties

Property code	Value	Unit	Source
gf	-172.62	kJ/mol	Joback Method
hf	-314.00	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	42.24	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.752		Crippen Method
mcvol	95.030	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	431.63	K	Joback Method
tc	626.00	K	Joback Method
tf	288.04	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.66	J/mol×K	431.63	Joback Method
cpg	170.10	J/mol×K	464.03	Joback Method
cpg	176.24	J/mol×K	496.42	Joback Method
cpg	182.09	J/mol×K	528.82	Joback Method
cpg	187.65	J/mol×K	561.21	Joback Method
cpg	192.93	J/mol×K	593.61	Joback Method
cpg	197.92	J/mol×K	626.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	328.70	K	2.00	NIST Webbook

Sources

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=C13698163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume