

Ethane, 1,1-dichloro-1-nitro-

Other names:	Ethide 1,1-Dichloro-1-nitroethane Dichloronitroethane 1,1-Dichlor-1-nitroaethan 1,1-Dicloro-1-nitroetano 1,1-Dichloor-1-nitroethaan UN 2650 NSC 6283 1-Nitro-1,1-dichloroethane
Inchi:	InChI=1S/C2H3Cl2NO2/c1-2(3,4)5(6)7/h1H3
InchiKey:	OQOGEOLRYAOSKO-UHFFFAOYSA-N
Formula:	C2H3Cl2NO2
SMILES:	CC(Cl)(Cl)[N+](=O)[O-]
Mol. weight [g/mol]:	143.96
CAS:	594-72-9

Physical Properties

Property code	Value	Unit	Source
gf	-19.51	kJ/mol	Joback Method
hf	-135.60	kJ/mol	Joback Method
hfus	13.28	kJ/mol	Joback Method
hvap	44.11	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.414		Crippen Method
mcvol	80.940	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
tb	396.70	K	NIST Webbook
tc	710.91	K	Joback Method
tf	318.17	K	Joback Method
vc	0.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	140.60	J/mol×K	468.63	Joback Method
cpg	146.77	J/mol×K	509.01	Joback Method
cpg	152.32	J/mol×K	549.39	Joback Method
cpg	157.30	J/mol×K	589.77	Joback Method
cpg	161.76	J/mol×K	630.15	Joback Method
cpg	165.75	J/mol×K	670.53	Joback Method
cpg	169.31	J/mol×K	710.91	Joback Method

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=C594729&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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