Ethane, 1-chloro-2-nitro-

Other names: 2-Chloronitroethane
Inchi: InChI=1S/C2H4ClNO2/c3-1-2-4(5)6/h1-2H2
InchiKey: XMZRJPITAOAPLJ-UHFFFAOYSA-N
Formula: C2H4ClNO2
SMILES: O=[N+]([O-])CCCl
Mol. weight [g/mol]: 109.51
CAS: 625-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-10.42	kJ/mol	Joback Method
hf	-111.11	kJ/mol	Joback Method
hfus	16.49	kJ/mol	Joback Method
hvap	41.02	kJ/mol	Joback Method
log10ws	-0.90		Crippen Method
logp	0.502		Crippen Method
mcvol	68.700	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
tb	446.70	K	NIST Webbook
tc	653.95	K	Joback Method
tf	285.83	K	Joback Method
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.47	J/mol×K	434.43	Joback Method
cpg	124.29	J/mol×K	471.02	Joback Method
cpg	129.77	J/mol×K	507.60	Joback Method
cpg	134.93	J/mol×K	544.19	Joback Method
cpg	139.78	J/mol×K	580.78	Joback Method
cpg	144.32	J/mol×K	617.36	Joback Method
cpg	148.59	J/mol×K	653.95	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.20	K	9.60	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=C625478&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