Ethane, 1-chloro-1,1-dinitro-

Inchi: InChI=1S/C2H3ClN2O4/c1-2(3,4(6)7)5(8)9/h1H3
InchiKey: WCEVKBJRFBEDHR-UHFFFAOYSA-N
Formula: C2H3ClN2O4
SMILES: CC(Cl)([N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 154.51
CAS: 2972-95-4

Physical Properties

Property code	Value	Unit	Source
gf	27.97	kJ/mol	Joback Method
hf	-113.00	kJ/mol	NIST Webbook
hfl	-156.00	kJ/mol	NIST Webbook
hfus	20.44	kJ/mol	Joback Method
hvap	43.50	kJ/mol	NIST Webbook
log10ws	-2.08		Crippen Method
logp	0.452		Crippen Method
mcvol	86.120	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
tb	583.04	K	Joback Method
tc	851.83	K	Joback Method
tf	431.86	K	Joback Method
vc	0.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.50	J/mol×K	583.04	Joback Method
cpg	192.04	J/mol×K	627.84	Joback Method
cpg	197.85	J/mol×K	672.64	Joback Method
cpg	202.99	J/mol×K	717.44	Joback Method
cpg	207.54	J/mol×K	762.23	Joback Method
cpg	211.57	J/mol×K	807.03	Joback Method
cpg	215.15	J/mol×K	851.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2972954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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