Ethanol, 2-chloro-2,2-dinitro-

Inchi: InChI=1S/C2H3ClN2O5/c3-2(1-6,4(7)8)5(9)10/h6H,1H2
InchiKey: XQYDERLCYFKQIS-UHFFFAOYSA-N
Formula: C2H3ClN2O5
SMILES: O=[N+]([O-])C(Cl)(CO)[N+](=O)[O-]
Mol. weight [g/mol]: 170.51
CAS: 918-53-6

Physical Properties

Property code	Value	Unit	Source
gf	-108.85	kJ/mol	Joback Method
hf	-282.85	kJ/mol	Joback Method
hfs	-248.30	kJ/mol	NIST Webbook
hfus	24.53	kJ/mol	Joback Method
hvap	73.00	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	-0.575		Crippen Method
mcvol	91.990	ml/mol	McGowan Method
pc	5809.41	kPa	Joback Method
tb	675.22	K	Joback Method
tc	917.87	K	Joback Method
tf	492.68	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.55	J/mol×K	675.22	Joback Method
cpg	220.43	J/mol×K	715.66	Joback Method
cpg	224.79	J/mol×K	756.10	Joback Method
cpg	228.69	J/mol×K	796.54	Joback Method
cpg	232.19	J/mol×K	836.99	Joback Method
cpg	235.35	J/mol×K	877.43	Joback Method
cpg	238.21	J/mol×K	917.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C918536&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
hfs:	Solid 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