2-Nitro-2-ethyl-1,3-propanediol

Other names:	1,3-Propanediol, 2-ethyl-2-nitro-
	2-Ethyl-2-nitropropanediol
	2-Ethyl-2-nitro-1,3-propanediol
	NEPD
	2-ethyl-2-nitropropane-1,3-diol
Inchi:	InChI=1S/C5H11NO4/c1-2-5(3-7,4-8)6(9)10/h7-8H,2-4H2,1H3
InchiKey:	YADISKICBOYXFS-UHFFFAOYSA-N
Formula:	C5H11NO4
SMILES:	CCC(CO)(CO)[N+](=O)[O-]
Mol. weight [g/mol]:	149.15
CAS:	597-09-1

Physical Properties

Property code	Value	Unit	Source
chs	-2938.00	kJ/mol	NIST Webbook
chs	-2931.90 ± 1.30	kJ/mol	NIST Webbook
gf	-244.03	kJ/mol	Joback Method
hf	-470.50	kJ/mol	Joback Method
hfs	-607.70 ± 1.40	kJ/mol	NIST Webbook
hfs	-601.20	kJ/mol	NIST Webbook
hfus	20.83	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	-0.603		Crippen Method
mcvol	110.470	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	646.77	K	Joback Method
tc	838.44	K	Joback Method
tf	413.78	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	298.50	J/mol×K	646.77	Joback Method
cpg	306.20	J/mol×K	678.72	Joback Method
cpg	313.42	J/mol×K	710.66	Joback Method
cpg	320.20	J/mol×K	742.61	Joback Method
cpg	326.56	J/mol×K	774.55	Joback Method
cpg	332.54	J/mol×K	806.50	Joback Method
cpg	338.16	J/mol×K	838.44	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C597091&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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