1,3-Propanediol, 2-methyl-2-nitro-, dinitrate

Other names: 2-Nitro-2-methyl-1,3-propanediol dinitrate
Inchi: InChI=1S/C4H7N3O8/c1-4(5(8)9,2-14-6(10)11)3-15-7(12)13/h2-3H2,1H3
InchiKey: PNEVRNLRPGLOIP-UHFFFAOYSA-N
Formula: C4H7N3O8
SMILES: CC(CO[N+](=O)[O-])(CO[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]: 225.11
CAS: 4055-94-1

Physical Properties

Property code	Value	Unit	Source
chs	-2200.00 ± 2.20	kJ/mol	NIST Webbook
chs	-2203.20	kJ/mol	NIST Webbook
gf	-117.71	kJ/mol	Joback Method
hf	-431.36	kJ/mol	Joback Method
hfs	-371.30	kJ/mol	NIST Webbook
hfs	-374.00 ± 2.20	kJ/mol	NIST Webbook
hfus	35.16	kJ/mol	Joback Method
hvap	77.80	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	-0.562		Crippen Method
mcvol	131.220	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	788.05	K	Joback Method
tc	1051.26	K	Joback Method
tf	612.55	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.34	J/mol×K	788.05	Joback Method
cpg	380.33	J/mol×K	831.92	Joback Method
cpg	387.41	J/mol×K	875.79	Joback Method
cpg	393.63	J/mol×K	919.66	Joback Method

cpg	399.00	J/mol×K	963.53	Joback Method
cpg	403.57	J/mol×K	1007.39	Joback Method
cpg	407.35	J/mol×K	1051.26	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=C4055941&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