Nitroisobutanetriol trinitrate

Other names:	1,3-Propanediol, 2-nitro-2-[(nitrooxy)methyl]-, dinitrate (ester)
	1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-, trinitrate (ester)
	Nitroisobutylglycerol trinitrate
	1,3-Propanediol, 2-nitro-2-[(nitrooxy)methyl]-, dinitrate
	1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-, trinitrate
	Nitroisobutyl glyceryl trinitrate
	Nitroisobutylglycol trinitrate
	Trimethylolnitromethane trinitrate
	1,3-Propanediol, 2-nitro-2-[(nitrooxy)methyl]-, 1,3-dinitrate
	2-nitro-2-[(nitrooxy)methyl]propane-1,3-diyl dinitrate
Inchi:	InChI=1S/C4H6N4O11/c9-5(10)4(1-17-6(11)12,2-18-7(13)14)3-19-8(15)16/h1-3H2
InchiKey:	LQVCBLBPWSZOPA-UHFFFAOYSA-N
Formula:	C4H6N4O11
SMILES:	O=[N+]([O-])OCC(CO[N+](=O)[O-])(CO[N+](=O)[O-])[N+](=O)[O-]
Mol. weight [g/mol]:	286.11
CAS:	20820-44-4

Physical Properties

Property code	Value	Unit	Source
chs	-2205.20	kJ/mol	NIST Webbook
gf	-187.16	kJ/mol	Joback Method
hf	-574.34	kJ/mol	Joback Method
hfs	-226.00	kJ/mol	NIST Webbook
hfus	47.71	kJ/mol	Joback Method
hvap	96.80	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	-1.373		Crippen Method
mcvol	154.510	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	962.31	K	Joback Method
tc	1234.98	K	Joback Method
tf	778.39	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.63	J/mol×K	962.31	Joback Method
cpg	468.30	J/mol×K	1007.76	Joback Method
cpg	471.82	J/mol×K	1053.20	Joback Method
cpg	474.22	J/mol×K	1098.65	Joback Method
cpg	475.50	J/mol×K	1144.09	Joback Method
cpg	475.67	J/mol×K	1189.54	Joback Method
cpg	474.76	J/mol×K	1234.98	Joback Method
hvapt	72.90	kJ/mol	333.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20820444&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

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
hvapt: Enthalpy of vaporization at a given temperature
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