1,3-Propanediol, 2-nitro-2-[(nitrooxy)methyl]-, dinitrate (ester)

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

Physical Properties

Property code	Value	Unit	Source
chs	-2205.20	kJ/mol	NIST Webbook
hf	-254.88	kJ/mol	Cheméo Relay (1.0)
hfs	-226.00	kJ/mol	NIST Webbook
hfus	47.71	kJ/mol	Joback Method
hvap	96.29	kJ/mol	Cheméo Relay (1.0)
ie	11.24	eV	Cheméo Relay (1.0)
log10ws	-3.26		Cheméo Relay (1.0)
logp	-1.373		Crippen Method
mcvol	154.510	ml/mol	McGowan Method
tb	512.82	K	Cheméo Relay (1.0)
tf	391.38	K	Cheméo Relay (1.0)

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20820444&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point