1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-

Other names:	Isobutylglycerol, nitro-
	Methane, trimethylolnitro-
	Nitroisobutylglycerol
	Nitrotris(hydroxymethyl)methane
	Trihydroxymethylnitromethane
	Trimethylolnitromethane
	Tris Nitro
	Tris(hydroxymethyl)nitromethane
	1,1,1-Tris(hydroxymethyl)nitromethane
	2-(Hydroxymethyl)-2-nitropropanediol
	2-(Hydroxymethyl)-2-nitro-1,3-propanediol
	Cimcool wafers
	2-(Hydroxymethyl)-2-nitropropane-1,3-diol
	2-Nitro-2-(hydroxymethyl)-1,3-propanediol
	Nitrotrimethylolmethane
	NSC 17675
	nitromethylidynetrimethanol
Inchi:	InChI=1S/C4H9NO5/c6-1-4(2-7,3-8)5(9)10/h6-8H,1-3H2
InchiKey:	OLQJQHSAWMFDJE-UHFFFAOYSA-N
Formula:	C4H9NO5
SMILES:	O=[N+]([O-])C(CO)(CO)CO
Mol. weight [g/mol]:	151.12
CAS:	126-11-4

Physical Properties

Property code	Value	Unit	Source
chs	-2131.00 ± 3.10	kJ/mol	NIST Webbook
chs	-2118.00	kJ/mol	NIST Webbook
gf	-389.27	kJ/mol	Joback Method
hf	-602.09	kJ/mol	Joback Method
hfs	-742.20	kJ/mol	NIST Webbook
hfs	-729.40 ± 3.10	kJ/mol	NIST Webbook
hfus	22.33	kJ/mol	Joback Method
hvap	89.83	kJ/mol	Joback Method
log10ws	0.52		Crippen Method
logp	-2.021		Crippen Method
mcvol	102.250	ml/mol	McGowan Method

pc	5962.94	kPa	Joback Method
tb	716.07	K	Joback Method
tc	902.57	K	Joback Method
tf	463.33	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.64	J/mol×K	716.07	Joback Method
cpg	294.26	J/mol×K	747.15	Joback Method
cpg	299.53	J/mol×K	778.24	Joback Method
cpg	304.47	J/mol×K	809.32	Joback Method
cpg	309.12	J/mol×K	840.40	Joback Method
cpg	313.50	J/mol×K	871.49	Joback Method
cpg	317.65	J/mol×K	902.57	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=C126114&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