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

Other names:	1,3-Propanediol, 2-(hydroxymethyl)-2-methyl-, trinitrate
	Metriol trinitrate
	Trimethylolethane trinitrate
	Tris(hydroxymethyl)ethane trinitrate
	TMETN
	1,1,1-Trimethylolethane trinitrate
	2-Methyl-2-hydroxymethyl-1,3-propanediol trinitrate
	2-Methyl-2-nitro-oxymethyltrimethylene dinitrate
	1,3-Propanediol, 2-methyl-2-[(nitrooxy)methyl]-, dinitrate
	2-Methyl-2-[(nitrooxy)methyl]propane-1,3-diyl dinitrate
Inchi:	InChI=1S/C5H9N3O9/c1-5(2-15-6(9)10,3-16-7(11)12)4-17-8(13)14/h2-4H2,1H3
InchiKey:	IPPYBNCEPZCLNI-UHFFFAOYSA-N
Formula:	C5H9N3O9
SMILES:	CC(CO[N+](=O)[O-])(CO[N+](=O)[O-])CO[N+](=O)[O-]
Mol. weight [g/mol]:	255.14
CAS:	3032-55-1

Physical Properties

Property code	Value	Unit	Source
chl	-2811.00	kJ/mol	NIST Webbook
gf	-214.29	kJ/mol	Joback Method
hf	-584.22	kJ/mol	Joback Method
hfs	-450.20	kJ/mol	NIST Webbook
hfus	38.94	kJ/mol	Joback Method
hvap	88.20 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.16		Crippen Method
logp	-0.382		Crippen Method
mcvol	151.180	ml/mol	McGowan Method
pc	3484.76	kPa	Joback Method
rinpol	1529.00		NIST Webbook
rinpol	1529.00		NIST Webbook
tb	833.35	K	Joback Method
tc	1086.71	K	Joback Method
tf	646.05	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.14	J/mol×K	833.35	Joback Method
cpg	454.41	J/mol×K	875.58	Joback Method
cpg	461.67	J/mol×K	917.80	Joback Method
cpg	467.93	J/mol×K	960.03	Joback Method
cpg	473.20	J/mol×K	1002.26	Joback Method
cpg	477.48	J/mol×K	1044.49	Joback Method
cpg	480.78	J/mol×K	1086.71	Joback Method
hvapt	88.10	kJ/mol	322.00	NIST Webbook

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=C3032551&Units=SI

Legend

chl: Standard liquid 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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume