1,3-Propanediol, dinitrate

Other names:	Trimethylene dinitrate
	Trimethylene nitrate
	1,3-Propylene glycol dinitrate
Inchi:	InChI=1S/C3H6N2O6/c6-4(7)10-2-1-3-11-5(8)9/h1-3H2
InchiKey:	KOSAMXZBGUIISK-UHFFFAOYSA-N
Formula:	C3H6N2O6
SMILES:	O=[N+]([O-])OCCCO[N+](=O)[O-]
Mol. weight [g/mol]:	166.09
CAS:	3457-90-7

Physical Properties

Property code	Value	Unit	Source
chl	-1743.00	kJ/mol	NIST Webbook
gf	-164.52	kJ/mol	Joback Method
hf	-391.21	kJ/mol	Joback Method
hfus	28.62	kJ/mol	Joback Method
hvap	60.27	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	-0.207		Crippen Method
mcvol	99.710	ml/mol	McGowan Method
pc	4351.13	kPa	Joback Method
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
tb	616.56	K	Joback Method
tc	851.72	K	Joback Method
tf	455.25	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.17	J/mol×K	812.52	Joback Method
cpg	245.92	J/mol×K	616.56	Joback Method

cpg	254.21	J/mol×K	655.75	Joback Method
cpg	262.00	J/mol×K	694.95	Joback Method
cpg	269.26	J/mol×K	734.14	Joback Method
cpg	275.99	J/mol×K	773.33	Joback Method
cpg	287.78	J/mol×K	851.72	Joback Method
hvapt	74.30 ± 4.60	kJ/mol	303.00	NIST Webbook

Sources

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=C3457907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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