1,2-Propanediol, dinitrate

Other names:	1,2-PROPYLENE GLYCOL DINITRATE
	1,2-Propanediol, 1,2-dinitrate
	ISOPROPYLENE NITRATE
	NSC 62614
	PGDN
	PROPYLENE DINITRATE
	PROPYLENE GLYCOL DINITRATE
	Propylene glycol 1,2-dinitrate
	Propylene nitrate
	propane-1,2-diyl dinitrate
Inchi:	InChI=1S/C3H6N2O6/c1-3(11-5(8)9)2-10-4(6)7/h3H,2H2,1H3
InchiKey:	PSXCGTLGGVDWFU-UHFFFAOYSA-N
Formula:	C3H6N2O6
SMILES:	CC(CO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]:	166.09
CAS:	6423-43-4

Physical Properties

Property code	Value	Unit	Source
gf	-166.96	kJ/mol	Joback Method
hf	-396.49	kJ/mol	Joback Method
hfs	-296.90 ± 9.30	kJ/mol	NIST Webbook
hfus	25.10	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-1.51		Crippen Method
logp	-0.209		Crippen Method
mcvol	99.710	ml/mol	McGowan Method
pc	4397.41	kPa	Joback Method
rinpol	1004.00		NIST Webbook
rinpol	1004.00		NIST Webbook
tb	616.12	K	Joback Method
tc	856.44	K	Joback Method
tf	440.25	K	Joback Method
vc	0.398	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.49	J/mol×K	816.38	Joback Method
cpg	246.46	J/mol×K	616.12	Joback Method
cpg	254.98	J/mol×K	656.17	Joback Method
cpg	262.96	J/mol×K	696.23	Joback Method
cpg	270.39	J/mol×K	736.28	Joback Method
cpg	277.23	J/mol×K	776.33	Joback Method
cpg	289.14	J/mol×K	856.44	Joback Method
hvapt	63.80	kJ/mol	308.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6423434&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
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1429
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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