

1,2,3-Propanetriol, 1,3-dinitrate

Other names:	Glycerol, 1,3-dinitrate 1,3-Dinitroglycerin 1,3-Glyceryl dinitrate 1,3-DNG
Inchi:	InChI=1S/C3H6N2O7/c6-3(1-11-4(7)8)2-12-5(9)10/h3,6H,1-2H2
InchiKey:	ASIGVDLTBLZXNC-UHFFFAOYSA-N
Formula:	C3H6N2O7
SMILES:	O=[N+](([O-])OCC(O)CO[N+](=O)[O-])
Mol. weight [g/mol]:	182.09
CAS:	623-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-303.78	kJ/mol	Joback Method
hf	-548.72	kJ/mol	Joback Method
hfl	-477.00 ± 3.00	kJ/mol	NIST Webbook
hfus	29.19	kJ/mol	Joback Method
hvap	76.56	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	-1.236		Crippen Method
mcvol	105.580	ml/mol	McGowan Method
pc	4987.39	kPa	Joback Method
tb	708.30	K	Joback Method
tc	929.01	K	Joback Method
tf	501.07	K	Joback Method
vc	0.416	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.85	J/mol×K	708.30	Joback Method
cpg	289.73	J/mol×K	745.09	Joback Method
cpg	296.09	J/mol×K	781.87	Joback Method
cpg	301.94	J/mol×K	818.66	Joback Method

cpg	307.25	J/mol×K	855.44	Joback Method
cpg	312.02	J/mol×K	892.23	Joback Method
cpg	316.24	J/mol×K	929.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	389.20	K	0.08	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C623870&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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