1,2-Propanediol, 3,3'-oxydi-, tetranitrate

Other names: Diglycerol tetranitrate
Tetranitro diglycerin
Inchi: InChI=1S/C6H10N4O13/c11-7(12)20-3-5(22-9(15)16)1-19-2-6(23-10(17)18)4-21-8(13)14
InchiKey: SKKBQEZMHMDRLE-UHFFFAOYSA-N
Formula: C6H10N4O13
SMILES: O=[N+]([O-])OCC(COCC(CO[N+](=O)[O-])O[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 346.16
CAS: 20600-96-8

Physical Properties

Property code	Value	Unit	Source
chl	-3161.90	kJ/mol	NIST Webbook
gf	-388.04	kJ/mol	Joback Method
hf	-881.87	kJ/mol	Joback Method
hfus	55.63	kJ/mol	Joback Method
hvap	106.59	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	-1.427		Crippen Method
mcvol	194.430	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	1055.26	K	Joback Method
tc	1313.31	K	Joback Method
tf	812.97	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.81	J/mol×K	1055.26	Joback Method
cpg	614.95	J/mol×K	1098.27	Joback Method
cpg	615.19	J/mol×K	1141.28	Joback Method
cpg	613.46	J/mol×K	1184.28	Joback Method
cpg	609.69	J/mol×K	1227.29	Joback Method
cpg	603.83	J/mol×K	1270.30	Joback Method

cpg	595.81	J/mol×K	1313.31	Joback Method

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=C20600968&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
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