1,2,5-Pentanetriol trinitrate

Inchi: InChI=1S/C5H9N3O9/c9-6(10)15-3-1-2-5(17-8(13)14)4-16-7(11)12/h5H,1-4H2
InchiKey: NOTDFOCRTLYINY-UHFFFAOYSA-N
Formula: C5H9N3O9
SMILES: O=[N+]([O-])OCCCC(CO[N+](=O)[O-])O[N+](=O)[O-]
Mol. weight [g/mol]: 255.14
CAS: 98071-55-7

Physical Properties

Property code	Value	Unit	Source
chl	-2814.00	kJ/mol	NIST Webbook
gf	-219.57	kJ/mol	Joback Method
hf	-580.75	kJ/mol	Joback Method
hfus	42.83	kJ/mol	Joback Method
hvap	83.34	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	-0.240		Crippen Method
mcvol	151.180	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	836.14	K	Joback Method
tc	1081.51	K	Joback Method
tf	628.63	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.12	J/mol×K	1040.61	Joback Method
cpg	444.79	J/mol×K	836.14	Joback Method
cpg	453.14	J/mol×K	877.03	Joback Method
cpg	460.47	J/mol×K	917.93	Joback Method
cpg	466.76	J/mol×K	958.82	Joback Method
cpg	471.98	J/mol×K	999.72	Joback Method
cpg	479.15	J/mol×K	1081.51	Joback Method
hvapt	41.70 ± 2.10	kJ/mol	303.00	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=C98071557&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume