Pentaerythritol tetraacetate

Other names:	1,3-Propanediol, 2,2-bis[(acetyloxy)methyl]-, 1,3-diacetate
	1,3-Propanediol, 2,2-bis[(acetyloxy)methyl]-, diacetate
	2,2-Bis((acetyloxy)methyl)-1,3-propanediol diacetate
	NSC 1841
	Normo-level
	Normosterol
	PAG
	Pentaerythritole tetraacetate
	Pentaerythrityl tetraacetate
	Pentaerythrityl tetracetate
	T. A. P. E.
	TAPE
	Tetraacetil pentoetriol
	Tetraacetyl pentestriol
	[3-acetyloxy-2,2-bis(acetyloxymethyl)propyl] acetate
Inchi:	InChI=1S/C13H20O8/c1-9(14)18-5-13(6-19-10(2)15,7-20-11(3)16)8-21-12(4)17/h5-8H2,1
InchiKey:	OUHCZCFQVONTOC-UHFFFAOYSA-N
Formula:	C13H20O8
SMILES:	CC(=O)OCC(COC(C)=O)(COC(C)=O)COC(C)=O
Mol. weight [g/mol]:	304.29
CAS:	597-71-7

Physical Properties

Property code	Value	Unit	Source
gf	-874.26	kJ/mol	Joback Method
hf	-1299.60	kJ/mol	Joback Method
hfus	33.16	kJ/mol	Joback Method
hvap	79.86	kJ/mol	Joback Method
log10ws	-1.57		Aqueous Solubility Prediction Method
logp	0.225		Crippen Method
mcvol	223.790	ml/mol	McGowan Method
pc	1952.68	kPa	Joback Method
tb	798.77	K	Joback Method
tc	996.87	K	Joback Method
tf	356.65	K	Aqueous Solubility Prediction Method

vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.71	J/mol×K	798.77	Joback Method
cpg	713.47	J/mol×K	963.85	Joback Method
cpg	705.05	J/mol×K	930.83	Joback Method
cpg	695.66	J/mol×K	897.82	Joback Method
cpg	685.30	J/mol×K	864.80	Joback Method
cpg	673.98	J/mol×K	831.79	Joback Method
cpg	720.90	J/mol×K	996.87	Joback Method
dvisc	0.0000597	Pa×s	798.77	Joback Method
dvisc	0.0000762	Pa×s	753.53	Joback Method
dvisc	0.0001003	Pa×s	708.29	Joback Method
dvisc	0.0001372	Pa×s	663.05	Joback Method
dvisc	0.0001964	Pa×s	617.81	Joback Method
dvisc	0.0002975	Pa×s	572.57	Joback Method
dvisc	0.0004840	Pa×s	527.33	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C597717&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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