Mannitol, hexakis(trichloroacetate)

Inchi: InChI=1S/C18H8Cl18O12/c19-13(20,21)7(37)43-1-3(45-9(39)15(25,26)27)5(47-11(41)17
InchiKey: AVWKGFLULWRTFJ-UHFFFAOYSA-N
Formula: C18H8Cl18O12
SMILES: O=C(OCC(OC(=O)C(Cl)(Cl)Cl)C(OC(=O)C(Cl)(Cl)Cl)C(OC(=O)C(Cl)(Cl)Cl)C(COC(=O)C
Mol. weight [g/mol]: 1054.40
CAS: 133227-56-2

Physical Properties

Property code	Value	Unit	Source
gf	-1510.30	kJ/mol	Joback Method
hf	-2240.59	kJ/mol	Joback Method
hfus	76.07	kJ/mol	Joback Method
hvap	180.20	kJ/mol	Joback Method
log10ws	-10.35		Crippen Method
logp	7.941		Crippen Method
mcvol	529.440	ml/mol	McGowan Method
pc	982.69	kPa	Joback Method
tb	1721.58	K	Joback Method
tc	2193.65	K	Joback Method
tf	1218.66	K	Joback Method
vc	1.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.73	J/mol×K	1721.58	Joback Method
cpg	1423.02	J/mol×K	2114.97	Joback Method
cpg	1360.66	J/mol×K	2036.29	Joback Method
cpg	1309.76	J/mol×K	1957.62	Joback Method
cpg	1269.10	J/mol×K	1878.94	Joback Method
cpg	1237.49	J/mol×K	1800.26	Joback Method
cpg	1498.03	J/mol×K	2193.65	Joback Method
dvisc	1.5986796e-08	Pa×s	1721.58	Joback Method
dvisc	2.0824815e-08	Pa×s	1637.76	Joback Method

dvisc	2.7911790e-08	Pa×s	1553.94	Joback Method
dvisc	3.8681185e-08	Pa×s	1470.12	Joback Method
dvisc	5.5763313e-08	Pa×s	1386.30	Joback Method
dvisc	8.4264087e-08	Pa×s	1302.48	Joback Method
dvisc	0.0000001	Pa×s	1218.66	Joback Method

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=C133227562&Units=SI

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