D-Glucitol, hexaacetate

Other names:	Glucitol, hexaacetate, D-
	Hexa-O-acetylglucitol
	Sorbitol hexaacetate
	D-Sorbitol hexaacetate
	Hexaacetylsorbitol
	Glucitol hexaacetate
	hexa-O-acetyl-D-glucitol
Inchi:	InChI=1S/C18H26O12/c1-9(19)25-7-15(27-11(3)21)17(29-13(5)23)18(30-14(6)24)16(28-
InchiKey:	NJVBTKVPPOFGAT-UHFFFAOYSA-N
Formula:	C18H26O12
SMILES:	CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]:	434.39
CAS:	7208-47-1

Physical Properties

Property code	Value	Unit	Source
gf	-1312.60	kJ/mol	Joback Method
hf	-1904.77	kJ/mol	Joback Method
hfus	45.01	kJ/mol	Joback Method
hvap	109.05	kJ/mol	Joback Method
log10ws	-0.98		Crippen Method
logp	-0.161		Crippen Method
mcvol	309.120	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
tb	1067.22	K	Joback Method
tc	1308.46	K	Joback Method
tf	372.00 ± 3.00	K	NIST Webbook
vc	1.163	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1009.61	J/mol×K	1067.22	Joback Method
cpg	1009.62	J/mol×K	1268.25	Joback Method

cpg	1015.04	J/mol×K	1228.05	Joback Method
cpg	1017.68	J/mol×K	1187.84	Joback Method
cpg	1017.61	J/mol×K	1147.63	Joback Method
cpg	1014.89	J/mol×K	1107.43	Joback Method
cpg	1001.34	J/mol×K	1308.46	Joback Method
dvisc	0.0000110	Pa×s	1067.22	Joback Method
dvisc	0.0000145	Pa×s	1000.28	Joback Method
dvisc	0.0000198	Pa×s	933.34	Joback Method
dvisc	0.0000284	Pa×s	866.40	Joback Method
dvisc	0.0000433	Pa×s	799.46	Joback Method
dvisc	0.0000714	Pa×s	732.52	Joback Method
dvisc	0.0001300	Pa×s	665.58	Joback Method

Sources

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=C7208471&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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