mannitol, acetylated

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

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
rinpol	2054.20		NIST Webbook
tb	1067.22	K	Joback Method
tc	1308.46	K	Joback Method
tf	665.58	K	Joback Method
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:	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=R488981&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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