Sorbitol, 3,6-dimethyl, acetylated

Inchi: InChI=1S/C16H26O10/c1-9(17)23-8-14(25-11(3)19)15(22-6)16(26-12(4)20)13(7-21-5)24
InchiKey: BWFYMIDEWZXNAH-UGUYLWEFSA-N
Formula: C16H26O10
SMILES: COCC(OC(C)=O)C(OC(C)=O)C(OC)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 378.37

Physical Properties

Property code	Value	Unit	Source
gf	-1071.60	kJ/mol	Joback Method
hf	-1638.33	kJ/mol	Joback Method
hfus	36.63	kJ/mol	Joback Method
hvap	91.10	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.006		Crippen Method
mcvol	277.800	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2128.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	913.72	K	Joback Method
tc	1121.04	K	Joback Method
tf	543.18	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.98	J/mol×K	913.72	Joback Method
cpg	898.98	J/mol×K	948.27	Joback Method
cpg	909.42	J/mol×K	982.83	Joback Method
cpg	918.25	J/mol×K	1017.38	Joback Method
cpg	925.43	J/mol×K	1051.93	Joback Method
cpg	930.92	J/mol×K	1086.48	Joback Method
cpg	934.66	J/mol×K	1121.04	Joback Method

dvisc	0.0002856	Pa×s	543.18	Joback Method
dvisc	0.0001429	Pa×s	604.94	Joback Method
dvisc	0.0000813	Pa×s	666.69	Joback Method
dvisc	0.0000508	Pa×s	728.45	Joback Method
dvisc	0.0000342	Pa×s	790.21	Joback Method
dvisc	0.0000244	Pa×s	851.96	Joback Method
dvisc	0.0000182	Pa×s	913.72	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=R527754&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume