Sorbitol, 3-methyl, acetylated

Inchi: InChI=1S/C17H26O11/c1-9(18)24-7-14(26-11(3)20)16(23-6)17(28-13(5)22)15(27-12(4)2
InchiKey: RFZVFYLLLYGOTQ-YVSFHVDLSA-N
Formula: C17H26O11
SMILES: COC(C(COC(C)=O)OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 406.38

Physical Properties

Property code	Value	Unit	Source
gf	-1192.10	kJ/mol	Joback Method
hf	-1771.55	kJ/mol	Joback Method
hfus	40.82	kJ/mol	Joback Method
hvap	100.07	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	-0.077		Crippen Method
mcvol	293.460	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2108.00		NIST Webbook
rinpol	2101.00		NIST Webbook
rinpol	2108.00		NIST Webbook
tb	990.47	K	Joback Method
tc	1212.63	K	Joback Method
tf	604.38	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.08	J/mol×K	990.47	Joback Method
cpg	961.23	J/mol×K	1027.50	Joback Method
cpg	968.40	J/mol×K	1064.52	Joback Method
cpg	973.52	J/mol×K	1101.55	Joback Method
cpg	976.55	J/mol×K	1138.58	Joback Method
cpg	977.42	J/mol×K	1175.61	Joback Method
cpg	976.08	J/mol×K	1212.63	Joback Method

dvisc	0.0001910	Pa×s	604.38	Joback Method
dvisc	0.0001006	Pa×s	668.73	Joback Method
dvisc	0.0000593	Pa×s	733.08	Joback Method
dvisc	0.0000381	Pa×s	797.42	Joback Method
dvisc	0.0000261	Pa×s	861.77	Joback Method
dvisc	0.0000189	Pa×s	926.12	Joback Method
dvisc	0.0000142	Pa×s	990.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R527789&Units=SI
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

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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