2,3,4,6-Tetramethyl-1-acetylglucoside (A)

Inchi: InChI=1S/C12H22O7/c1-7(13)18-12-11(17-5)10(16-4)9(15-3)8(19-12)6-14-2/h8-12H,6H2
InchiKey: XMEWOWGGNTUINQ-AYQOGSFCSA-N
Formula: C12H22O7
SMILES: COCC1OC(OC(C)=O)C(OC)C(OC)C1OC
Mol. weight [g/mol]: 278.30

Physical Properties

Property code	Value	Unit	Source
gf	-696.27	kJ/mol	Joback Method
hf	-1223.73	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	64.80	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	-0.034		Crippen Method
mcvol	205.870	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1396.00		NIST Webbook
tb	667.75	K	Joback Method
tc	859.74	K	Joback Method
tf	403.07	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.02	J/mol×K	667.75	Joback Method
cpg	629.55	J/mol×K	699.75	Joback Method
cpg	647.16	J/mol×K	731.75	Joback Method
cpg	663.78	J/mol×K	763.75	Joback Method
cpg	679.38	J/mol×K	795.74	Joback Method

cpg	693.88	J/mol×K	827.74	Joback Method
cpg	707.26	J/mol×K	859.74	Joback Method
dvisc	0.0007221	Pa×s	403.07	Joback Method
dvisc	0.0004813	Pa×s	447.18	Joback Method
dvisc	0.0003451	Pa×s	491.30	Joback Method
dvisc	0.0002613	Pa×s	535.41	Joback Method
dvisc	0.0002065	Pa×s	579.52	Joback Method
dvisc	0.0001686	Pa×s	623.64	Joback Method
dvisc	0.0001415	Pa×s	667.75	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=R117441&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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