2,6-Dimethyl-1,3,4-triacetylglucoside (A)

Inchi: InChI=1S/C14H22O9/c1-7(15)20-11-10(6-18-4)23-14(22-9(3)17)13(19-5)12(11)21-8(2)16
InchiKey: OTGRTMDUFIMZLJ-ARDLJMPDSA-N
Formula: C14H22O9
SMILES: COCC1OC(OC(C)=O)C(OC)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 334.32

Physical Properties

Property code	Value	Unit	Source
gf	-937.27	kJ/mol	Joback Method
hf	-1490.17	kJ/mol	Joback Method
hfus	46.85	kJ/mol	Joback Method
hvap	82.75	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	-0.201		Crippen Method
mcvol	237.190	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1706.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	821.25	K	Joback Method
tc	1024.83	K	Joback Method
tf	525.47	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.99	J/mol×K	821.25	Joback Method
cpg	784.28	J/mol×K	855.18	Joback Method
cpg	798.10	J/mol×K	889.11	Joback Method
cpg	810.41	J/mol×K	923.04	Joback Method
cpg	821.15	J/mol×K	956.97	Joback Method
cpg	830.24	J/mol×K	990.90	Joback Method

cpg	837.63	J/mol×K	1024.83	Joback Method
dvisc	0.0006037	Pa×s	525.47	Joback Method
dvisc	0.0004122	Pa×s	574.77	Joback Method
dvisc	0.0002989	Pa×s	624.06	Joback Method
dvisc	0.0002272	Pa×s	673.36	Joback Method
dvisc	0.0001793	Pa×s	722.66	Joback Method
dvisc	0.0001458	Pa×s	771.95	Joback Method
dvisc	0.0001216	Pa×s	821.25	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R117525&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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