

3,4,6-Trimethyl-1,2-diacetylglucoside (A)

Inchi:	InChI=1S/C13H22O8/c1-7(14)19-12-11(18-5)10(17-4)9(6-16-3)21-13(12)20-8(2)15/h9-13
InchiKey:	RVVUVVKNALXNRR-XUJBLEAGSA-N
Formula:	C13H22O8
SMILES:	COCC1OC(OC(C)=O)C(OC(C)=O)C(OC)C1OC
Mol. weight [g/mol]:	306.31

Physical Properties

Property code	Value	Unit	Source
gf	-816.77	kJ/mol	Joback Method
hf	-1356.95	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	73.78	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	-0.118		Crippen Method
mvol	221.530	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1605.00		NIST Webbook
rinpol	1585.00		NIST Webbook
tb	744.50	K	Joback Method
tc	941.85	K	Joback Method
tf	464.27	K	Joback Method
vc	0.816	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.63	J/molxK	744.50	Joback Method
cpg	708.87	J/molxK	777.39	Joback Method
cpg	724.93	J/molxK	810.28	Joback Method
cpg	739.76	J/molxK	843.18	Joback Method
cpg	753.30	J/molxK	876.07	Joback Method
cpg	765.49	J/molxK	908.96	Joback Method
cpg	776.29	J/molxK	941.85	Joback Method
dvisc	0.0006779	Paxs	464.27	Joback Method

dvisc	0.0004575	Paxs	510.97	Joback Method
dvisc	0.0003297	Paxs	557.68	Joback Method
dvisc	0.0002500	Paxs	604.38	Joback Method
dvisc	0.0001972	Paxs	651.09	Joback Method
dvisc	0.0001606	Paxs	697.80	Joback Method
dvisc	0.0001342	Paxs	744.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R296410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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