

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

Inchi: InChI=1S/C14H22O9/c1-7(15)20-6-10-11(21-8(2)16)12(18-4)13(19-5)14(23-10)22-9(3)17
InchiKey: IFFLEPBFBCCLKRG-ARDLJMPDSA-N
Formula: C14H22O9
SMILES: COC1C(OC(C)=O)OC(COC(C)=O)C(OC(C)=O)C1OC
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	1702.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	821.25	K	Joback Method
tc	1024.83	K	Joback Method
tf	525.47	K	Joback Method
vc	0.877	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.99	J/molxK	821.25	Joback Method
cpg	784.28	J/molxK	855.18	Joback Method
cpg	798.10	J/molxK	889.11	Joback Method
cpg	810.41	J/molxK	923.04	Joback Method
cpg	821.15	J/molxK	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	Paxs	525.47	Joback Method
dvisc	0.0004122	Paxs	574.77	Joback Method
dvisc	0.0002989	Paxs	624.06	Joback Method
dvisc	0.0002272	Paxs	673.36	Joback Method
dvisc	0.0001793	Paxs	722.66	Joback Method
dvisc	0.0001458	Paxs	771.95	Joback Method
dvisc	0.0001216	Paxs	821.25	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R117481&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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