

2,4,6-Tri-O-acetyl-1,5-Anhydro-3-O-methyl-D-mann

Inchi: InChI=1S/C14H22O8/c1-7-12(18-5)13(21-9(3)16)11(20-8(2)15)6-19-14(7)22-10(4)17/h7,
InchiKey: BZJZPFTWQPRJQQ-UHFFFAOYSA-N
Formula: C14H22O8
SMILES: COC1C(C)C(OC(C)=O)OCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 318.32

Physical Properties

Property code	Value	Unit	Source
gf	-844.37	kJ/mol	Joback Method
hf	-1364.11	kJ/mol	Joback Method
hfus	43.56	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-1.04		Crippen Method
logp	0.420		Crippen Method
mvol	231.320	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	1820.22		NIST Webbook
tb	803.10	K	Joback Method
tc	1011.07	K	Joback Method
tf	499.72	K	Joback Method
vc	0.852	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.89	J/molxK	803.10	Joback Method
cpg	760.19	J/molxK	837.76	Joback Method
cpg	775.00	J/molxK	872.42	Joback Method
cpg	788.25	J/molxK	907.09	Joback Method
cpg	799.89	J/molxK	941.75	Joback Method
cpg	809.87	J/molxK	976.41	Joback Method
cpg	818.11	J/molxK	1011.07	Joback Method
dvisc	0.0007014	Paxs	499.72	Joback Method
dvisc	0.0004487	Paxs	550.28	Joback Method

dvisc	0.0003095	Paxs	600.85	Joback Method
dvisc	0.0002261	Paxs	651.41	Joback Method
dvisc	0.0001728	Paxs	701.97	Joback Method
dvisc	0.0001370	Paxs	752.54	Joback Method
dvisc	0.0001118	Paxs	803.10	Joback Method

Sources

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=R320637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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