

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

Inchi:	InChI=1S/C13H20O8/c1-7(14)19-11-6-18-10(5-17-4)12(20-8(2)15)13(11)21-9(3)16/h10-1
InchiKey:	PLVOJUFADFXQMF-UHFFFAOYSA-N
Formula:	C13H20O8
SMILES:	COCC1OCC(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	304.29

Physical Properties

Property code	Value	Unit	Source
gf	-832.98	kJ/mol	Joback Method
hf	-1316.97	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	78.42	kJ/mol	Joback Method
log10ws	-0.37		Crippen Method
logp	-0.173		Crippen Method
mcvol	217.230	ml/mol	McGowan Method
pc	1978.82	kPa	Joback Method
rinpol	1745.51		NIST Webbook
rinpol	1745.51		NIST Webbook
tb	780.62	K	Joback Method
tc	985.59	K	Joback Method
tf	496.21	K	Joback Method
vc	0.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.74	J/molxK	780.62	Joback Method
cpg	743.76	J/molxK	951.43	Joback Method
cpg	733.66	J/molxK	917.27	Joback Method
cpg	722.16	J/molxK	883.11	Joback Method
cpg	709.31	J/molxK	848.94	Joback Method
cpg	695.16	J/molxK	814.78	Joback Method
cpg	752.43	J/molxK	985.59	Joback Method
dvisc	0.0001413	Paxs	780.62	Joback Method

dvisc	0.0001719	Paxs	733.22	Joback Method
dvisc	0.0002150	Paxs	685.82	Joback Method
dvisc	0.0002778	Paxs	638.41	Joback Method
dvisc	0.0003742	Paxs	591.01	Joback Method
dvisc	0.0005308	Paxs	543.61	Joback Method
dvisc	0.0008049	Paxs	496.21	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=R179890&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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