2,3,4-Tri-O-acetyl-1,5-anhydro-6-O-methyl-D-gluci

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	1750.40		NIST Webbook
rinpol	1750.40		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/mol×K	780.62	Joback Method
cpg	695.16	J/mol×K	814.78	Joback Method
cpg	709.31	J/mol×K	848.94	Joback Method
cpg	722.16	J/mol×K	883.11	Joback Method
cpg	733.66	J/mol×K	917.27	Joback Method
cpg	743.76	J/mol×K	951.43	Joback Method
cpg	752.43	J/mol×K	985.59	Joback Method
dvisc	0.0008049	Pa×s	496.21	Joback Method

dvisc	0.0005308	Pa×s	543.61	Joback Method
dvisc	0.0003742	Pa×s	591.01	Joback Method
dvisc	0.0002778	Pa×s	638.41	Joback Method
dvisc	0.0002150	Pa×s	685.82	Joback Method
dvisc	0.0001719	Pa×s	733.22	Joback Method
dvisc	0.0001413	Pa×s	780.62	Joback Method

Sources

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=U357219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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