

2,3-Di-O-acetyl-1,4-anhydro-5-O-methyl-L-fucitol

Inchi:	InChI=1S/C11H18O6/c1-6(14-4)10-11(17-8(3)13)9(5-15-10)16-7(2)12/h6,9-11H,5H2,1-4
InchiKey:	HZYGGBFYNBEJCR-UHFFFAOYSA-N
Formula:	C11H18O6
SMILES:	COC(C)C1OCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	246.26

Physical Properties

Property code	Value	Unit	Source
gf	-598.53	kJ/mol	Joback Method
hf	-1009.67	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.283		Crippen Method
mcvol	181.610	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinsol	1484.40		NIST Webbook
tb	658.53	K	Joback Method
tc	860.46	K	Joback Method
tf	394.27	K	Joback Method
vc	0.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.37	J/molxK	658.53	Joback Method
cpg	533.50	J/molxK	692.19	Joback Method
cpg	548.74	J/molxK	725.84	Joback Method
cpg	563.07	J/molxK	759.50	Joback Method
cpg	576.46	J/molxK	793.15	Joback Method
cpg	588.90	J/molxK	826.81	Joback Method
cpg	600.36	J/molxK	860.46	Joback Method
dvisc	0.0015656	Paxs	394.27	Joback Method
dvisc	0.0009684	Paxs	438.31	Joback Method

dvisc	0.0006539	Paxs	482.36	Joback Method
dvisc	0.0004715	Paxs	526.40	Joback Method
dvisc	0.0003576	Paxs	570.44	Joback Method
dvisc	0.0002822	Paxs	614.49	Joback Method
dvisc	0.0002298	Paxs	658.53	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=U357238&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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