

2,3,4-tri-O-acetyl-1,5-anhydro-D-fucitol

Inchi:	InChI=1S/C12H18O7/c1-6-11(18-8(3)14)12(19-9(4)15)10(5-16-6)17-7(2)13/h6,10-12H,5H
InchiKey:	QPTFIDGGNPUDEM-VYLNZQIESA-N
Formula:	C12H18O7
SMILES:	CC(=O)OC1COC(C)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	274.27

Physical Properties

Property code	Value	Unit	Source
gf	-736.40	kJ/mol	Joback Method
hf	-1164.11	kJ/mol	Joback Method
hfus	38.22	kJ/mol	Joback Method
hvap	73.79	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.200		Crippen Method
mcvol	197.270	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1588.91		NIST Webbook
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tb	735.32	K	Joback Method
tc	943.30	K	Joback Method
tf	462.71	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.91	J/molxK	735.32	Joback Method
cpg	662.85	J/molxK	908.64	Joback Method
cpg	651.88	J/molxK	873.97	Joback Method
cpg	639.66	J/molxK	839.31	Joback Method
cpg	626.24	J/molxK	804.65	Joback Method
cpg	611.64	J/molxK	769.98	Joback Method
cpg	672.54	J/molxK	943.30	Joback Method
dvisc	0.0002054	Paxs	735.32	Joback Method

dvisc	0.0002491	Paxs	689.88	Joback Method
dvisc	0.0003104	Paxs	644.45	Joback Method
dvisc	0.0003999	Paxs	599.01	Joback Method
dvisc	0.0005372	Paxs	553.58	Joback Method
dvisc	0.0007606	Paxs	508.15	Joback Method
dvisc	0.0011531	Paxs	462.71	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=R221619&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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