

2,4-Di-O-acetyl-1,5-Anhydro-3-O-methyl-L-rhamnitol

Inchi:	InChI=1S/C11H18O6/c1-6-10(17-8(3)13)11(14-4)9(5-15-6)16-7(2)12/h6,9-11H,5H2,1-4H
InchiKey:	WKCHTFIVXNUTCJ-JGBZZBSPSA-N
Formula:	C11H18O6
SMILES:	COC1C(OC(C)=O)COC(C)C1OC(C)=O
Mol. weight [g/mol]:	246.26

Physical Properties

Property code	Value	Unit	Source
gf	-615.90	kJ/mol	Joback Method
hf	-1030.89	kJ/mol	Joback Method
hfus	34.03	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-0.67		Crippen Method
logp	0.283		Crippen Method
mcvol	181.610	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinsol	1490.06		NIST Webbook
tb	658.57	K	Joback Method
tc	862.68	K	Joback Method
tf	401.51	K	Joback Method
vc	0.668	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.31	J/molxK	658.57	Joback Method
cpg	538.33	J/molxK	692.59	Joback Method
cpg	554.40	J/molxK	726.61	Joback Method
cpg	569.49	J/molxK	760.63	Joback Method
cpg	583.56	J/molxK	794.64	Joback Method
cpg	596.58	J/molxK	828.66	Joback Method
cpg	608.52	J/molxK	862.68	Joback Method
dvisc	0.0012794	Paxs	401.51	Joback Method
dvisc	0.0008278	Paxs	444.35	Joback Method

dvisc	0.0005783	Paxs	487.20	Joback Method
dvisc	0.0004281	Paxs	530.04	Joback Method
dvisc	0.0003314	Paxs	572.88	Joback Method
dvisc	0.0002659	Paxs	615.73	Joback Method
dvisc	0.0002196	Paxs	658.57	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=R182935&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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