

2-O-acetyl-1,4-Anhydro-3,5-di-O-methyl-D-ribitol

Inchi: InChI=1S/C9H16O5/c1-6(10)14-8-5-13-7(4-11-2)9(8)12-3/h7-9H,4-5H2,1-3H3/t7-,8+,9-/m
InchiKey: GIPDUYRMXHDLKV-YIZRAAEISA-N
Formula: C9H16O5
SMILES: COCC1OCC(OC(C)=O)C1OC
Mol. weight [g/mol]: 204.22

Physical Properties

Property code	Value	Unit	Source
hfus	28.29	kJ/mol	Joback Method
logp	-0.022		Crippen Method
mcvol	151.860	ml/mol	McGowan Method
rinpol	1320.42		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.71	J/mol×K	559.34	Joback Method
cpg	477.80	J/mol×K	755.50	Joback Method
cpg	465.53	J/mol×K	722.81	Joback Method
cpg	452.54	J/mol×K	690.12	Joback Method
cpg	438.84	J/mol×K	657.42	Joback Method
cpg	424.45	J/mol×K	624.73	Joback Method
cpg	409.40	J/mol×K	592.03	Joback Method
dvisc	0.0005045	Pa×s	448.07	Joback Method
dvisc	0.0002695	Pa×s	559.34	Joback Method
dvisc	0.0003224	Pa×s	522.25	Joback Method
dvisc	0.0003965	Pa×s	485.16	Joback Method
dvisc	0.0014298	Pa×s	336.80	Joback Method
dvisc	0.0006706	Pa×s	410.98	Joback Method
dvisc	0.0009431	Pa×s	373.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R180642&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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