

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C9H16O5/c1-6(10)14-9-7(12-3)5-13-8(9)4-11-2/h7-9H,4-5H2,1-3H3/t7-,8+,9-/m

XGUPLFWZEJKRNN-HRDYMLBCSA-N

C9H16O5

COCC1OCC(OC)C1OC(C)=O

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

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R180662&Units=SI

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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