

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

Other names:	3-O-Acetyl-1,4-Anhydro-2,5-di-O-methyl-D-xylitol
Inchi:	InChI=1S/C9H16O5/c1-6(10)14-9-7(12-3)5-13-8(9)4-11-2/h7-9H,4-5H2,1-3H3
InchiKey:	XGUPLFWZEJKRNN-UHFFFAOYSA-N
Formula:	C9H16O5
SMILES:	COCC1OCC(OC)C1OC(C)=O
Mol. weight [g/mol]:	204.22

Physical Properties

Property code	Value	Unit	Source
gf	-484.01	kJ/mol	Joback Method
hf	-850.53	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	-0.022		Crippen Method
mvol	151.860	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	1320.82		NIST Webbook
rinpol	1320.82		NIST Webbook
tb	559.34	K	Joback Method
tc	755.50	K	Joback Method
tf	336.80	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.71	J/molxK	559.34	Joback Method
cpg	465.53	J/molxK	722.81	Joback Method
cpg	452.54	J/molxK	690.12	Joback Method
cpg	438.84	J/molxK	657.42	Joback Method
cpg	424.45	J/molxK	624.73	Joback Method
cpg	409.40	J/molxK	592.03	Joback Method
cpg	477.80	J/molxK	755.50	Joback Method

dvisc	0.0002695	Paxs	559.34	Joback Method
dvisc	0.0003224	Paxs	522.25	Joback Method
dvisc	0.0003965	Paxs	485.16	Joback Method
dvisc	0.0005045	Paxs	448.07	Joback Method
dvisc	0.0006706	Paxs	410.98	Joback Method
dvisc	0.0009431	Paxs	373.89	Joback Method
dvisc	0.0014298	Paxs	336.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357228&Units=SI
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

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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