

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

Inchi:	InChI=1S/C10H16O6/c1-6(11)15-9-5-14-4-8(13-3)10(9)16-7(2)12/h8-10H,4-5H2,1-3H3/t
InchiKey:	MVVNLUDKWSGDPL-KXUCPTDWSA-N
Formula:	C10H16O6
SMILES:	COC1COCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	232.23

Physical Properties

Property code	Value	Unit	Source
gf	-616.61	kJ/mol	Joback Method
hf	-989.91	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	62.90	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.105		Crippen Method
mvol	167.520	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1439.24		NIST Webbook
rinpol	1439.24		NIST Webbook
tb	640.36	K	Joback Method
tc	847.49	K	Joback Method
tf	394.48	K	Joback Method
vc	0.614	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.79	J/molxK	640.36	Joback Method
cpg	482.87	J/molxK	674.88	Joback Method
cpg	498.07	J/molxK	709.40	Joback Method
cpg	512.36	J/molxK	743.92	Joback Method
cpg	525.70	J/molxK	778.44	Joback Method
cpg	538.07	J/molxK	812.97	Joback Method
cpg	549.43	J/molxK	847.49	Joback Method
dvisc	0.0013874	Paxs	394.48	Joback Method

dvisc	0.0008679	Paxs	435.46	Joback Method
dvisc	0.0005885	Paxs	476.44	Joback Method
dvisc	0.0004244	Paxs	517.42	Joback Method
dvisc	0.0003211	Paxs	558.40	Joback Method
dvisc	0.0002524	Paxs	599.38	Joback Method
dvisc	0.0002046	Paxs	640.36	Joback Method

Sources

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=R194626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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