

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

Inchi: InChI=1S/C10H16O6/c1-6(11)14-5-9-10(16-7(2)12)8(13-3)4-15-9/h8-10H,4-5H2,1-3H3/t8
InchiKey: OYQRUEYSACUGFJ-KXUCPTDWSA-N
Formula: C10H16O6
SMILES: COC1COC(COC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 232.23

Physical Properties

Property code	Value	Unit	Source
hfus	32.47	kJ/mol	Joback Method
logp	-0.105		Crippen Method
mcvol	167.520	ml/mol	McGowan Method
rinpol	1492.57		NIST Webbook
rinpol	1492.57		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.89	J/mol×K	636.09	Joback Method
cpg	480.18	J/mol×K	669.58	Joback Method
cpg	494.68	J/mol×K	703.07	Joback Method
cpg	508.36	J/mol×K	736.57	Joback Method
cpg	521.20	J/mol×K	770.06	Joback Method
cpg	533.18	J/mol×K	803.55	Joback Method
cpg	544.28	J/mol×K	837.04	Joback Method
dvisc	0.0014137	Pa×s	398.00	Joback Method
dvisc	0.0009483	Pa×s	437.68	Joback Method
dvisc	0.0006797	Pa×s	477.36	Joback Method
dvisc	0.0005128	Pa×s	517.05	Joback Method
dvisc	0.0004027	Pa×s	556.73	Joback Method
dvisc	0.0003266	Pa×s	596.41	Joback Method
dvisc	0.0002719	Pa×s	636.09	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R180657&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

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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