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

Inchi: InChI=1S/C8H16O4/c1-9-4-7-8(11-3)6(10-2)5-12-7/h6-8H,4-5H2,1-3H3/t6-,7+,8-/m1/s1
InchiKey: PFPWLRZFWHVNMO-GJMOJQLCSA-N
Formula: C8H16O4
SMILES: COCC1OCC(OC)C1OC
Mol. weight [g/mol]: 176.21

Physical Properties

Property code	Value	Unit	Source
hfus	24.10	kJ/mol	Joback Method
ie	9.13	eV	Cheméo Relay (1.0)
logp	0.062		Crippen Method
mcvol	136.200	ml/mol	McGowan Method
rinpol	1215.73		NIST Webbook
rinpol	1215.73		NIST Webbook
tb	505.98	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.69	J/mol×K	482.59	Joback Method
cpg	339.18	J/mol×K	514.20	Joback Method
cpg	354.19	J/mol×K	545.80	Joback Method
cpg	368.68	J/mol×K	577.41	Joback Method
cpg	382.64	J/mol×K	609.02	Joback Method
cpg	396.06	J/mol×K	640.62	Joback Method
cpg	408.90	J/mol×K	672.23	Joback Method
dvisc	0.0012924	Pa×s	275.60	Joback Method
dvisc	0.0008383	Pa×s	310.10	Joback Method
dvisc	0.0005930	Pa×s	344.60	Joback Method
dvisc	0.0004467	Pa×s	379.10	Joback Method
dvisc	0.0003528	Pa×s	413.59	Joback Method
dvisc	0.0002890	Pa×s	448.09	Joback Method
dvisc	0.0002436	Pa×s	482.59	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R180602&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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature