

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

Inchi:	InChI=1S/C8H16O4/c1-9-6-4-12-5-7(10-2)8(6)11-3/h6-8H,4-5H2,1-3H3/t6-,7+,8-
InchiKey:	DKQVTQIPWUFZRF-RNLVFAQGSA-N
Formula:	C8H16O4
SMILES:	COC1COCC(OC)C1OC
Mol. weight [g/mol]:	176.21

Physical Properties

Property code	Value	Unit	Source
gf	-375.61	kJ/mol	Joback Method
hf	-723.47	kJ/mol	Joback Method
hfus	22.00	kJ/mol	Joback Method
hvap	44.95	kJ/mol	Joback Method
log10ws	0.25		Crippen Method
logp	0.062		Crippen Method
mcvol	136.200	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1223.26		NIST Webbook
rinpol	1223.26		NIST Webbook
tb	486.86	K	Joback Method
tc	683.58	K	Joback Method
tf	272.08	K	Joback Method
vc	0.489	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.57	J/molxK	486.86	Joback Method
cpg	340.03	J/molxK	519.65	Joback Method
cpg	355.96	J/molxK	552.43	Joback Method
cpg	371.34	J/molxK	585.22	Joback Method
cpg	386.13	J/molxK	618.01	Joback Method
cpg	400.30	J/molxK	650.80	Joback Method
cpg	413.82	J/molxK	683.58	Joback Method
dvisc	0.0016357	Paxs	272.08	Joback Method

dvisc	0.0009442	Paxs	307.88	Joback Method
dvisc	0.0006112	Paxs	343.67	Joback Method
dvisc	0.0004294	Paxs	379.47	Joback Method
dvisc	0.0003207	Paxs	415.27	Joback Method
dvisc	0.0002508	Paxs	451.06	Joback Method
dvisc	0.0002034	Paxs	486.86	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=R194577&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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