

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

Inchi:	InChI=1S/C11H16O7/c1-6(12)15-4-9-11(18-8(3)14)10(5-16-9)17-7(2)13/h9-11H,4-5H2,1
InchiKey:	AGTSQJAVJCFOSJ-AXFHLTTASA-N
Formula:	C11H16O7
SMILES:	CC(=O)OCC1OCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	260.24

Physical Properties

Property code	Value	Unit	Source
gf	-725.01	kJ/mol	Joback Method
hf	-1116.97	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	71.70	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	-0.188		Crippen Method
mcvol	183.180	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1617.28		NIST Webbook
tb	712.84	K	Joback Method
tc	917.89	K	Joback Method
tf	459.20	K	Joback Method
vc	0.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.86	J/molxK	712.84	Joback Method
cpg	550.23	J/molxK	747.02	Joback Method
cpg	563.65	J/molxK	781.19	Joback Method
cpg	576.10	J/molxK	815.37	Joback Method
cpg	587.55	J/molxK	849.54	Joback Method
cpg	597.98	J/molxK	883.72	Joback Method
cpg	607.37	J/molxK	917.89	Joback Method
dvisc	0.0013024	Paxs	459.20	Joback Method
dvisc	0.0008869	Paxs	501.47	Joback Method

dvisc	0.0006411	Paxs	543.75	Joback Method
dvisc	0.0004856	Paxs	586.02	Joback Method
dvisc	0.0003819	Paxs	628.29	Joback Method
dvisc	0.0003095	Paxs	670.57	Joback Method
dvisc	0.0002572	Paxs	712.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R180617&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

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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