

1,5-Anhydro-6-o-acetyl-2,3,4-tri-o-methyl-d-manni

Other names:	6-O-Acetyl-1,5-anhydro-2,3,4-tri-O-methyl-D-mannitol
Inchi:	InChI=1S/C11H20O6/c1-7(12)16-6-9-11(15-4)10(14-3)8(13-2)5-17-9/h8-11H,5-6H2,1-4H
InchiKey:	BHKQJVAXJLYKPU-CHWFTXMASA-N
Formula:	C11H20O6
SMILES:	CO[C@@H]1[C@H](OC)[C@@H](OC)CO[C@H]1COC(C)=O
Mol. weight [g/mol]:	248.28

Physical Properties

Property code	Value	Unit	Source
hfus	33.62	kJ/mol	Joback Method
logp	-0.007		Crippen Method
mcvol	185.910	ml/mol	McGowan Method
rinpol	1603.36		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.85	J/mol×K	627.12	Joback Method
cpg	543.85	J/mol×K	659.71	Joback Method
cpg	561.01	J/mol×K	692.29	Joback Method
cpg	577.30	J/mol×K	724.88	Joback Method
cpg	592.68	J/mol×K	757.46	Joback Method
cpg	607.10	J/mol×K	790.05	Joback Method
cpg	620.52	J/mol×K	822.64	Joback Method
dvisc	0.0010224	Pa×s	373.81	Joback Method
dvisc	0.0006464	Pa×s	416.03	Joback Method
dvisc	0.0004447	Pa×s	458.25	Joback Method
dvisc	0.0003259	Pa×s	500.47	Joback Method
dvisc	0.0002506	Pa×s	542.68	Joback Method
dvisc	0.0002002	Pa×s	584.90	Joback Method
dvisc	0.0001648	Pa×s	627.12	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C93635962&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
rinpol:	Non-polar retention indices

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