

2,3,4-O-triacetyl-1,5-Anhydro-L-arabinitol

Inchi:	InChI=1S/C11H16O7/c1-6(12)16-9-4-15-5-10(17-7(2)13)11(9)18-8(3)14/h9-11H,4-5H2,1
InchiKey:	NEMMESQJOZVCAX-UWVGGGRQHSA-N
Formula:	C11H16O7
SMILES:	CC(=O)OC1COCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	260.24

Physical Properties

Property code	Value	Unit	Source
gf	-737.11	kJ/mol	Joback Method
hf	-1123.13	kJ/mol	Joback Method
hfus	34.56	kJ/mol	Joback Method
hvap	71.87	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	-0.188		Crippen Method
mcvol	183.180	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	1578.67		NIST Webbook
rinpol	1578.67		NIST Webbook
tb	717.11	K	Joback Method
tc	927.75	K	Joback Method
tf	455.68	K	Joback Method
vc	0.675	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.54	J/molxK	717.11	Joback Method
cpg	553.52	J/molxK	752.22	Joback Method
cpg	567.45	J/molxK	787.32	Joback Method
cpg	580.28	J/molxK	822.43	Joback Method
cpg	591.99	J/molxK	857.54	Joback Method
cpg	602.55	J/molxK	892.64	Joback Method
cpg	611.91	J/molxK	927.75	Joback Method
dvisc	0.0011838	Paxs	455.68	Joback Method

dvisc	0.0007610	Paxs	499.25	Joback Method
dvisc	0.0005252	Paxs	542.82	Joback Method
dvisc	0.0003830	Paxs	586.39	Joback Method
dvisc	0.0002918	Paxs	629.97	Joback Method
dvisc	0.0002302	Paxs	673.54	Joback Method
dvisc	0.0001870	Paxs	717.11	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R187410&Units=SI

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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