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-UWVGGRQHSA-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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0007610	Pa×s	499.25	Joback Method
dvisc	0.0005252	Pa×s	542.82	Joback Method
dvisc	0.0003830	Pa×s	586.39	Joback Method
dvisc	0.0002918	Pa×s	629.97	Joback Method
dvisc	0.0002302	Pa×s	673.54	Joback Method
dvisc	0.0001870	Pa×s	717.11	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=R187410&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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