

3,4-Di-O-acetyl-1,5-anhydro-2,6-di-O-methyl-D-glucopyranose

Inchi:	InChI=1S/C12H20O7/c1-7(13)18-11-9(16-4)6-17-10(5-15-3)12((11)19-8(2)14/h9-12H,5-6
InchiKey:	RMOCGTLPYRNXIM-UHFFFAOYSA-N
Formula:	C12H20O7
SMILES:	COCC1OCC(OC)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	276.28

Physical Properties

Property code	Value	Unit	Source
gf	-712.48	kJ/mol	Joback Method
hf	-1183.75	kJ/mol	Joback Method
hfus	37.81	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-0.17		Crippen Method
logp	-0.090		Crippen Method
mcvol	201.570	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1644.98		NIST Webbook
rinpol	1644.98		NIST Webbook
tb	703.87	K	Joback Method
tc	903.99	K	Joback Method
tf	435.01	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.82	J/molxK	703.87	Joback Method
cpg	620.83	J/molxK	737.22	Joback Method
cpg	636.79	J/molxK	770.58	Joback Method
cpg	651.67	J/molxK	803.93	Joback Method
cpg	665.42	J/molxK	837.28	Joback Method
cpg	678.02	J/molxK	870.64	Joback Method
cpg	689.40	J/molxK	903.99	Joback Method
dvisc	0.0009285	Paxs	435.01	Joback Method

dvisc	0.0006006	Paxs	479.82	Joback Method
dvisc	0.0004185	Paxs	524.63	Joback Method
dvisc	0.0003087	Paxs	569.44	Joback Method
dvisc	0.0002380	Paxs	614.25	Joback Method
dvisc	0.0001902	Paxs	659.06	Joback Method
dvisc	0.0001563	Paxs	703.87	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=U357216&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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