

«beta»-D-Glucopyranose, 1,6-anhydro-, triacetate

Other names:

Levoglucosan, triacetate
Triacetyllevoglucosan
1,6-Anhydro-«beta»-D-glucopyranose triacetate
6,8-Dioxabicyclo[3.2.1]octane, b-d-glucopyranose deriv.
1,6-Anhydro-b-d-glucopyranose triacetate
1,6-Anhydro-2,3,4-tri-O-acetyl-b-d-glucopyranose
2,3,4-Tri-O-acetyl-1,6-anhydro-b-d-glucopyranose
1,6-anhydro-«beta»-D-glucose triacetate

Inchi: InChI=1S/C12H16O8/c1-5(13)17-9-8-4-16-12(20-8)11(19-7(3)15)10(9)18-6(2)14/h8-12H,1

InchiKey: BAKQMOSGYGQJOJ-LVEVGFFFA-N

Formula: C12H16O8

SMILES: CC(=O)OC1C2COC(O2)C(OC(C)=O)C1OC(C)=O

Mol. weight [g/mol]: 288.25

CAS: 13242-55-2

Physical Properties

Property code	Value	Unit	Source
gf	-749.67	kJ/mol	Joback Method
hf	-1217.15	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	-0.463		Crippen Method
mcvol	192.280	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
tb	764.74	K	Joback Method
tc	977.29	K	Joback Method
tf	510.74	K	Joback Method
vc	0.717	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.07	J/mol×K	764.74	Joback Method

cpg	669.20	J/molxK	941.87	Joback Method
cpg	659.26	J/molxK	906.44	Joback Method
cpg	648.16	J/molxK	871.02	Joback Method
cpg	635.93	J/molxK	835.59	Joback Method
cpg	622.57	J/molxK	800.17	Joback Method
cpg	678.00	J/molxK	977.29	Joback Method
dvisc	0.0007516	Paxs	764.74	Joback Method
dvisc	0.0008529	Paxs	722.41	Joback Method
dvisc	0.0009833	Paxs	680.07	Joback Method
dvisc	0.0011552	Paxs	637.74	Joback Method
dvisc	0.0013887	Paxs	595.41	Joback Method
dvisc	0.0017170	Paxs	553.07	Joback Method
dvisc	0.0021990	Paxs	510.74	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=C13242552&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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