«alpha»-D-Glucofuranose, 1,2-O-(1-methylethylidene)-

Other names: 1,2-O-Isopropylidene-D-glucofuranose
1,2-O-Isopropylidene-«alpha»-D-glucofuranose
Glucofuranose, 1,2-O-isopropylidene-, «alpha»-D-
Furo[2,3-d]-1,3-dioxole, «alpha»-d-glucofuranose deriv.
Glucofuranose, 1,2-O-isopropylidene-
Glucofuranose, 1,2-O-isopropylidene-, alpha-d-
1,2-Mono-O-isopropylidene-«alpha»-d-glucofuranose
1,2-O-(1-Methylethylidene)-«alpha»-d-glucofuranose
1,2-O-Isopropylidene-alpha-d-glucofuranose
NSC 1697

Inchi: InChI=1S/C9H16O6/c1-9(2)14-7-5(12)6(4(11)3-10)13-8(7)15-9/h4-8,10-12H,3H2,1-2H3

InchiKey: BGGCXQKYCBBHAH-UHFFFAOYSA-N

Formula: C9H16O6

SMILES: CC1(C)OC2OC(C(O)CO)C(O)C2O1

Mol. weight [g/mol]: 220.22

CAS: 18549-40-1

Physical Properties

Property code	Value	Unit	Source
gf	-577.68	kJ/mol	Joback Method
hf	-999.56	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	96.90	kJ/mol	Joback Method
log10ws	-0.09		Crippen Method
logp	-1.423		Crippen Method
mcvol	151.170	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
tb	770.52	K	Joback Method
tc	958.67	K	Joback Method
tf	478.38	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.86	J/mol×K	770.52	Joback Method
cpg	522.86	J/mol×K	801.88	Joback Method
cpg	533.58	J/mol×K	833.24	Joback Method
cpg	544.09	J/mol×K	864.59	Joback Method
cpg	554.47	J/mol×K	895.95	Joback Method
cpg	564.82	J/mol×K	927.31	Joback Method
cpg	575.20	J/mol×K	958.67	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=C18549401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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