1,2:4,6-Di-O-isopropylidene-L-sorbopyranose

Other names: L-Sorbose, bis-O-(1-methylethylidene)-
Diacetone sorbose
Inchi: InChI=1S/C12H20O6/c1-10(2)15-6-12(18-10)9-8(13)7(5-14-12)16-11(3,4)17-9/h7-9,13H,
InchiKey: HIHGMQOBMJOZKO-UHFFFAOYSA-N
Formula: C12H20O6
SMILES: CC1(C)OC2COC3(COC(C)(C)O3)C(O1)C2O
Mol. weight [g/mol]: 260.28
CAS: 32717-65-0

Physical Properties

Property code	Value	Unit	Source
gf	-423.01	kJ/mol	Joback Method
hf	-924.78	kJ/mol	Joback Method
hfus	41.14	kJ/mol	Joback Method
hvap	77.58	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.377		Crippen Method
mcvol	182.580	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1534.00		NIST Webbook
tb	724.90	K	Joback Method
tc	951.13	K	Joback Method
tf	517.39	K	Joback Method
vc	0.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.64	J/mol×K	724.90	Joback Method
cpg	620.05	J/mol×K	762.61	Joback Method
cpg	637.43	J/mol×K	800.31	Joback Method
cpg	655.11	J/mol×K	838.02	Joback Method
cpg	673.46	J/mol×K	875.72	Joback Method

cpg	692.82	J/mol×K	913.43	Joback Method
cpg	713.54	J/mol×K	951.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C32717650&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume