1,2-5,6-Diacetone L-mannitol

Inchi: InChI=1S/C12H22O6/c1-11(2)15-5-7(17-11)9(13)10(14)8-6-16-12(3,4)18-8/h7-10,13-14H
InchiKey: ODYBCPSCYHAGHA-XKNYDFJKSA-N
Formula: C12H22O6
SMILES: CC1(C)OCC(C(O)C(O)C2COC(C)(C)O2)O1
Mol. weight [g/mol]: 262.30
CAS: 22323-78-0

Physical Properties

Property code	Value	Unit	Source
chs	-6397.30	kJ/mol	NIST Webbook
gf	-526.14	kJ/mol	Joback Method
hf	-1023.27	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	90.52	kJ/mol	Joback Method
log10ws	-1.17		Crippen Method
logp	0.011		Crippen Method
mcvol	193.440	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
tb	786.94	K	Joback Method
tc	991.90	K	Joback Method
tf	484.04	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.08	J/mol×K	786.94	Joback Method
cpg	665.63	J/mol×K	821.10	Joback Method
cpg	681.07	J/mol×K	855.26	Joback Method
cpg	696.60	J/mol×K	889.42	Joback Method
cpg	712.38	J/mol×K	923.58	Joback Method
cpg	728.58	J/mol×K	957.74	Joback Method
cpg	745.40	J/mol×K	991.90	Joback Method

Sources

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=C22323780&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
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