[2H]Glucitolamine hexaacetate

Inchi: InChI=1S/C18H27NO11/c1-9(20)19-15(7-26-10(2)21)17(29-13(5)24)18(30-14(6)25)16(28
InchiKey: TYXRQWOGEBZZOX-UHFFFAOYSA-N
Formula: C18H27NO11
SMILES: CC(=O)NC(COC(C)=O)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 433.41

Physical Properties

Property code	Value	Unit	Source
gf	-1118.21	kJ/mol	Joback Method
hf	-1719.08	kJ/mol	Joback Method
hfus	48.92	kJ/mol	Joback Method
hvap	113.07	kJ/mol	Joback Method
log10ws	-1.08		Crippen Method
logp	-0.588		Crippen Method
mcvol	313.230	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	2210.00		NIST Webbook
tb	1094.97	K	Joback Method
tc	1344.19	K	Joback Method
tf	696.01	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.83	J/mol×K	1094.97	Joback Method
cpg	1038.55	J/mol×K	1136.51	Joback Method
cpg	1040.68	J/mol×K	1178.04	Joback Method
cpg	1040.19	J/mol×K	1219.58	Joback Method
cpg	1037.02	J/mol×K	1261.11	Joback Method
cpg	1031.12	J/mol×K	1302.65	Joback Method
cpg	1022.43	J/mol×K	1344.19	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=R176346&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