d-inositol

Inchi: InChI=1S/C6H12O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-12H
InchiKey: PVTHJAPFENJVNC-UHFFFAOYSA-N
Formula: C6H12O6
SMILES: OC1C(O)C(O)C(O)C(O)C1O
Mol. weight [g/mol]: 180.16

Physical Properties

Property code	Value	Unit	Source
gf	-835.38	kJ/mol	Joback Method
hf	-1127.93	kJ/mol	Joback Method
hfus	33.01	kJ/mol	Joback Method
hvap	127.91	kJ/mol	Joback Method
log10ws	0.35		Estimated Solubility Method
log10ws	0.35		Aqueous Solubility Prediction Method
logp	-3.835		Crippen Method
mcvol	119.760	ml/mol	McGowan Method
pc	6921.35	kPa	Joback Method
tb	885.96	K	Joback Method
tc	1086.32	K	Joback Method
tf	522.65	K	Aqueous Solubility Prediction Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.69	J/mol×K	885.96	Joback Method
cpg	444.88	J/mol×K	919.35	Joback Method
cpg	451.35	J/mol×K	952.75	Joback Method
cpg	457.10	J/mol×K	986.14	Joback Method
cpg	462.12	J/mol×K	1019.53	Joback Method
cpg	466.41	J/mol×K	1052.93	Joback Method
cpg	469.97	J/mol×K	1086.32	Joback Method

dvisc	0.0001206	Pa×s	508.48	Joback Method
dvisc	0.0000136	Pa×s	571.39	Joback Method
dvisc	0.0000024	Pa×s	634.31	Joback Method
dvisc	0.0000006	Pa×s	697.22	Joback Method
dvisc	0.0000002	Pa×s	760.13	Joback Method
dvisc	6.1853059e-08	Pa×s	823.05	Joback Method
dvisc	2.5924234e-08	Pa×s	885.96	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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