Myo-inositol, hexaacetate

Other names:	Inositol, hexaacetate, myo- Mesoinositol hexaacetate Hexakis-O-acetyl-myo-inositol meso-inositol, acetylated
Inchi:	InChI=1S/C18H24O12/c1-7(19)25-13-14(26-8(2)20)16(28-10(4)22)18(30-12(6)24)17(29-
InchiKey:	SQUHHTBVTRBESD-UHFFFAOYSA-N
Formula:	C18H24O12
SMILES:	CC(=O)OC1C(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]:	432.38
CAS:	1254-38-2

Physical Properties

Property code	Value	Unit	Source
gf	-1316.94	kJ/mol	Joback Method
hf	-1931.03	kJ/mol	Joback Method
hfus	56.29	kJ/mol	Joback Method
hvap	109.48	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	-0.410		Crippen Method
mcvol	298.260	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinpol	2043.60		NIST Webbook
rinpol	2043.60		NIST Webbook
tb	1065.18	K	Joback Method
tc	1304.11	K	Joback Method
tf	711.76	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.39	J/mol×K	1065.18	Joback Method
cpg	1028.25	J/mol×K	1105.00	Joback Method
cpg	1028.90	J/mol×K	1144.82	Joback Method

cpg	1026.21	J/mol×K	1184.64	Joback Method
cpg	1020.07	J/mol×K	1224.46	Joback Method
cpg	1010.36	J/mol×K	1264.28	Joback Method
cpg	996.97	J/mol×K	1304.11	Joback Method
dvisc	0.0003354	Pa×s	711.76	Joback Method
dvisc	0.0002404	Pa×s	770.66	Joback Method
dvisc	0.0001807	Pa×s	829.57	Joback Method
dvisc	0.0001410	Pa×s	888.47	Joback Method
dvisc	0.0001135	Pa×s	947.37	Joback Method
dvisc	0.0000937	Pa×s	1006.28	Joback Method
dvisc	0.0000790	Pa×s	1065.18	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=C1254382&Units=SI

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