

Allo-Inositol

Other names:	Inositol, allo-
Inchi:	InChI=1S/C6H12O6/c7-1-2(8)4(10)6(12)5(11)3(1)9/h1-12H/t1-,2-,3-,4-,5-,6+
InchiKey:	CDAISMWEOUEBRE-OQYPVSDDSA-N
Formula:	C6H12O6
SMILES:	OC1C(O)C(O)C(O)C(O)C1O
Mol. weight [g/mol]:	180.16
CAS:	643-10-7

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	1.52		Crippen Method
logp	-3.835		Crippen Method
mcvol	119.760	ml/mol	McGowan Method
pc	6921.35	kPa	Joback Method
rinpol	1944.00		NIST Webbook
tb	885.96	K	Joback Method
tc	1086.32	K	Joback Method
tf	508.48	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0001206	Paxs	508.48	Joback Method
dvisc	0.0000136	Paxs	571.39	Joback Method
dvisc	0.0000024	Paxs	634.31	Joback Method
dvisc	0.0000006	Paxs	697.22	Joback Method
dvisc	0.0000002	Paxs	760.13	Joback Method
dvisc	6.1853059e-08	Paxs	823.05	Joback Method
dvisc	2.5924234e-08	Paxs	885.96	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=C643107&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
mvol:	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

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