Pinitol

Other names: D-pinitol
Inchi: InChI=1S/C7H14O6/c1-13-7-5(11)3(9)2(8)4(10)6(7)12/h2-12H,1H3/t2-,3-,4-,5-,6+,7+/m1/
InchiKey: DSCFFEYYQKSRSV-FQGZZYRYSA-N
Formula: C7H14O6
SMILES: COC1C(O)C(O)C(O)C(O)C1O
Mol. weight [g/mol]: 194.18
CAS: 484-68-4

Physical Properties

Property code	Value	Unit	Source
gf	-795.14	kJ/mol	Joback Method
hf	-1128.56	kJ/mol	Joback Method
hfus	32.70	kJ/mol	Joback Method
hvap	115.86	kJ/mol	Joback Method
log10ws	1.28		Crippen Method
logp	-3.180		Crippen Method
mcvol	133.850	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
rinpol	1880.00		NIST Webbook
tb	839.08	K	Joback Method
tc	1027.35	K	Joback Method
tf	481.16	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.97	J/mol×K	839.08	Joback Method
cpg	510.01	J/mol×K	995.97	Joback Method
cpg	504.32	J/mol×K	964.59	Joback Method
cpg	497.86	J/mol×K	933.21	Joback Method
cpg	490.64	J/mol×K	901.84	Joback Method
cpg	482.67	J/mol×K	870.46	Joback Method
cpg	514.93	J/mol×K	1027.35	Joback Method

dvisc	0.0000002	Pa×s	839.08	Joback Method
dvisc	0.0000004	Pa×s	779.43	Joback Method
dvisc	0.0000009	Pa×s	719.77	Joback Method
dvisc	0.0000027	Pa×s	660.12	Joback Method
dvisc	0.0000098	Pa×s	600.47	Joback Method
dvisc	0.0000472	Pa×s	540.81	Joback Method
dvisc	0.0003372	Pa×s	481.16	Joback Method

Sources

D-Pinitol Solubility in Supercritical CO2: Experimental Data and Correlation:	https://www.doi.org/10.1021/je0504257
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=C484684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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