2,3,4-Trimethyllevoglucosan

Other names: 1,6-Anhydro-«beta»-D-glucose, trimethyl ether
Inchi: InChI=1S/C9H16O5/c1-10-6-5-4-13-9(14-5)8(12-3)7(6)11-2/h5-9H,4H2,1-3H3
InchiKey: ZZSLTIGBKYUBSG-UHFFFAOYSA-N
Formula: C9H16O5
SMILES: COC1C2COC(O2)C(OC)C1OC
Mol. weight [g/mol]: 204.22
CAS: 2951-86-2

Physical Properties

Property code	Value	Unit	Source
gf	-388.17	kJ/mol	Joback Method
hf	-817.49	kJ/mol	Joback Method
hfus	33.87	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	0.13		Crippen Method
logp	-0.214		Crippen Method
mcvol	145.300	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1403.90		NIST Webbook
tb	534.49	K	Joback Method
tc	734.91	K	Joback Method
tf	327.14	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.34	J/mol×K	534.49	Joback Method
cpg	406.77	J/mol×K	567.89	Joback Method
cpg	423.44	J/mol×K	601.30	Joback Method
cpg	439.34	J/mol×K	634.70	Joback Method
cpg	454.47	J/mol×K	668.10	Joback Method
cpg	468.81	J/mol×K	701.51	Joback Method
cpg	482.37	J/mol×K	734.91	Joback Method

dvisc	0.0012049	Pa×s	327.14	Joback Method
dvisc	0.0010024	Pa×s	361.70	Joback Method
dvisc	0.0008612	Pa×s	396.26	Joback Method
dvisc	0.0007581	Pa×s	430.81	Joback Method
dvisc	0.0006801	Pa×s	465.37	Joback Method
dvisc	0.0006193	Pa×s	499.93	Joback Method
dvisc	0.0005709	Pa×s	534.49	Joback Method

Sources

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=C2951862&Units=SI
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
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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