

L-Sorbitol permethyl

Inchi:	InChI=1S/C12H26O6/c1-13-7-9(15-3)11(17-5)12(18-6)10(16-4)8-14-2/h9-12H,7-8H2,1-6
InchiKey:	UJQZVTQJKNAPOQ-UHFFFAOYSA-N
Formula:	C12H26O6
SMILES:	COCC(OC)C(OC)C(OC)C(COC)OC
Mol. weight [g/mol]:	266.33

Physical Properties

Property code	Value	Unit	Source
gf	-589.60	kJ/mol	Joback Method
hf	-1105.45	kJ/mol	Joback Method
hfus	19.87	kJ/mol	Joback Method
hvap	55.21	kJ/mol	Joback Method
log10ws	0.18		Crippen Method
logp	0.339		Crippen Method
mvol	215.160	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinpol	1491.00		NIST Webbook
rinpol	1491.00		NIST Webbook
tb	606.72	K	Joback Method
tc	778.56	K	Joback Method
tf	298.38	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.96	J/molxK	606.72	Joback Method
cpg	597.80	J/molxK	635.36	Joback Method
cpg	614.05	J/molxK	664.00	Joback Method
cpg	629.69	J/molxK	692.64	Joback Method
cpg	644.69	J/molxK	721.28	Joback Method
cpg	659.03	J/molxK	749.92	Joback Method
cpg	672.67	J/molxK	778.56	Joback Method
dvisc	0.0022252	Paxs	298.38	Joback Method

dvisc	0.0007085	Paxs	349.77	Joback Method
dvisc	0.0003024	Paxs	401.16	Joback Method
dvisc	0.0001566	Paxs	452.55	Joback Method
dvisc	0.0000928	Paxs	503.94	Joback Method
dvisc	0.0000606	Paxs	555.33	Joback Method
dvisc	0.0000425	Paxs	606.72	Joback Method

Sources

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=R71519&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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