

«beta»-D-Mannopyranoside, 1-cyclohexyl, permethylated

Inchi:	InChI=1S/C16H30O6/c1-17-10-12-13(18-2)14(19-3)15(20-4)16(22-12)21-11-8-6-5-7-9-1
InchiKey:	KBMAHMXTIVYWOQ-RBGFHDKUSA-N
Formula:	C16H30O6
SMILES:	COCC1OC(OC2CCCCC2)C(OC)C(OC)C1OC
Mol. weight [g/mol]:	318.41

Physical Properties

Property code	Value	Unit	Source
gf	-509.22	kJ/mol	Joback Method
hf	-1139.39	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	1.752		Crippen Method
mcvol	249.800	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	1908.00		NIST Webbook
rinpol	1908.00		NIST Webbook
tb	724.95	K	Joback Method
tc	928.67	K	Joback Method
tf	405.60	K	Joback Method
vc	0.904	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.66	J/mol×K	724.95	Joback Method
cpg	833.22	J/mol×K	758.90	Joback Method
cpg	855.24	J/mol×K	792.86	Joback Method
cpg	875.68	J/mol×K	826.81	Joback Method
cpg	894.49	J/mol×K	860.77	Joback Method
cpg	911.62	J/mol×K	894.72	Joback Method
cpg	927.04	J/mol×K	928.67	Joback Method
dvisc	0.0007721	Paxs	405.60	Joback Method

dvisc	0.0004469	Paxs	458.83	Joback Method
dvisc	0.0002898	Paxs	512.05	Joback Method
dvisc	0.0002039	Paxs	565.28	Joback Method
dvisc	0.0001524	Paxs	618.50	Joback Method
dvisc	0.0001193	Paxs	671.73	Joback Method
dvisc	0.0000968	Paxs	724.95	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=R549789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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