

«alpha»-D-Mannopyranoside, 1-butyl, permethylated

Inchi:	InChI=1S/C14H28O6/c1-6-7-8-19-14-13(18-5)12(17-4)11(16-3)10(20-14)9-15-2/h10-14H
InchiKey:	XXWYTNABLVGILP-ODXJTSPBSA-N
Formula:	C14H28O6
SMILES:	CCCCOC1OC(COC)C(OC)C(OC)C1OC
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-550.51	kJ/mol	Joback Method
hf	-1152.43	kJ/mol	Joback Method
hfus	42.05	kJ/mol	Joback Method
hvap	62.51	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.219		Crippen Method
mcvol	232.480	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinsol	1657.00		NIST Webbook
tb	659.64	K	Joback Method
tc	841.56	K	Joback Method
tf	375.68	K	Joback Method
vc	0.860	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.75	J/molxK	659.64	Joback Method
cpg	715.30	J/molxK	689.96	Joback Method
cpg	734.93	J/molxK	720.28	Joback Method
cpg	753.58	J/molxK	750.60	Joback Method
cpg	771.23	J/molxK	780.92	Joback Method
cpg	787.84	J/molxK	811.24	Joback Method
cpg	803.36	J/molxK	841.56	Joback Method
dvisc	0.0006855	Paxs	375.68	Joback Method
dvisc	0.0004257	Paxs	423.01	Joback Method

dvisc	0.0002910	Paxs	470.33	Joback Method
dvisc	0.0002132	Paxs	517.66	Joback Method
dvisc	0.0001646	Paxs	564.99	Joback Method
dvisc	0.0001323	Paxs	612.31	Joback Method
dvisc	0.0001097	Paxs	659.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R549625&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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