«beta»-D-Glucopyranoside, 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-HPCHECBXSA-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
rinpol	1704.00		NIST Webbook
rinpol	1704.00		NIST Webbook
tb	659.64	K	Joback Method
tc	841.56	K	Joback Method
tf	375.68	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.75	J/mol×K	659.64	Joback Method
cpg	715.30	J/mol×K	689.96	Joback Method
cpg	734.93	J/mol×K	720.28	Joback Method
cpg	753.58	J/mol×K	750.60	Joback Method
cpg	771.23	J/mol×K	780.92	Joback Method
cpg	787.84	J/mol×K	811.24	Joback Method
cpg	803.36	J/mol×K	841.56	Joback Method
dvisc	0.0006855	Pa×s	375.68	Joback Method

dvisc	0.0004257	Pa×s	423.01	Joback Method
dvisc	0.0002910	Pa×s	470.33	Joback Method
dvisc	0.0002132	Pa×s	517.66	Joback Method
dvisc	0.0001646	Pa×s	564.99	Joback Method
dvisc	0.0001323	Pa×s	612.31	Joback Method
dvisc	0.0001097	Pa×s	659.64	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R549729&Units=SI

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