

«beta»-D-Glucopyranoside, 1-(2-butyl), permethylated, # 1

Inchi: InChI=1S/C14H28O6/c1-7-9(2)19-14-13(18-6)12(17-5)11(16-4)10(20-14)8-15-3/h9-14H,7
InchiKey: XDPVZURCZKIZAJ-PMSMCTBISA-N
Formula: C14H28O6
SMILES: CCC(C)OC1OC(COC)C(OC)C(OC)C1OC
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
hfus	38.53	kJ/mol	Joback Method
logp	1.218		Crippen Method
mcvol	232.480	ml/mol	McGowan Method
rinpol	1576.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.13	J/mol×K	659.20	Joback Method
cpg	716.03	J/mol×K	689.99	Joback Method
cpg	735.97	J/mol×K	720.77	Joback Method
cpg	754.90	J/mol×K	751.56	Joback Method
cpg	772.79	J/mol×K	782.34	Joback Method
cpg	789.58	J/mol×K	813.13	Joback Method
cpg	805.25	J/mol×K	843.91	Joback Method
dvisc	0.0007948	Pa×s	360.68	Joback Method
dvisc	0.0004584	Pa×s	410.43	Joback Method
dvisc	0.0002978	Pa×s	460.19	Joback Method
dvisc	0.0002105	Pa×s	509.94	Joback Method
dvisc	0.0001582	Pa×s	559.69	Joback Method
dvisc	0.0001246	Pa×s	609.45	Joback Method
dvisc	0.0001017	Pa×s	659.20	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R549709&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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