«alpha»-D-Galactopyranoside, 1-cyclohexyl, permethylated

Inchi: InChI=1S/C16H30O6/c1-17-10-12-13(18-2)14(19-3)15(20-4)16(22-12)21-11-8-6-5-7-9-11

InchiKey: KBMAHMXTIVYWOQ-CWVYHPPDSA-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	1894.00		NIST Webbook
rinpol	1894.00		NIST Webbook
tb	724.95	K	Joback Method
tc	928.67	K	Joback Method
tf	405.60	K	Joback Method
vc	0.904	m3/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	Pa×s	405.60	Joback Method

dvisc	0.0004469	Pa×s	458.83	Joback Method
dvisc	0.0002898	Pa×s	512.05	Joback Method
dvisc	0.0002039	Pa×s	565.28	Joback Method
dvisc	0.0001524	Pa×s	618.50	Joback Method
dvisc	0.0001193	Pa×s	671.73	Joback Method
dvisc	0.0000968	Pa×s	724.95	Joback Method

Sources

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=R549536&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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