«alpha»-D-Mannopyranoside, permethylated

Inchi: InChI=1S/C11H22O6/c1-12-6-7-8(13-2)9(14-3)10(15-4)11(16-5)17-7/h7-11H,6H2,1-5H3/
InchiKey: ZYGZAHUNAGVTEC-FBDQPXRJSA-N
Formula: C11H22O6
SMILES: COCC1OC(OC)C(OC)C(OC)C1OC
Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-575.77	kJ/mol	Joback Method
hf	-1090.51	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	55.83	kJ/mol	Joback Method
log10ws	0.10		Crippen Method
logp	0.049		Crippen Method
mcvol	190.210	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	1447.00		NIST Webbook
rinpol	1447.00		NIST Webbook
tb	591.00	K	Joback Method
tc	777.61	K	Joback Method
tf	341.87	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.91	J/mol×K	591.00	Joback Method
cpg	548.07	J/mol×K	622.10	Joback Method
cpg	566.52	J/mol×K	653.20	Joback Method
cpg	584.22	J/mol×K	684.31	Joback Method
cpg	601.13	J/mol×K	715.41	Joback Method
cpg	617.19	J/mol×K	746.51	Joback Method
cpg	632.36	J/mol×K	777.61	Joback Method
dvisc	0.0007109	Pa×s	341.87	Joback Method

dvisc	0.0004684	Pa×s	383.39	Joback Method
dvisc	0.0003348	Pa×s	424.91	Joback Method
dvisc	0.0002541	Pa×s	466.44	Joback Method
dvisc	0.0002017	Pa×s	507.96	Joback Method
dvisc	0.0001658	Pa×s	549.48	Joback Method
dvisc	0.0001401	Pa×s	591.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R549645&Units=SI
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

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