Xylobiose, permethyl

Inchi: InChI=1S/C16H30O9/c1-17-9-7-24-16(14(21-5)11(9)18-2)25-10-8-23-15(22-6)13(20-4)12
InchiKey: DEILOTUZCRMGNS-XHJURHDUSA-N
Formula: C16H30O9
SMILES: COC1COC(OC2COC(OC)C(OC)C2OC)C(OC)C1OC
Mol. weight [g/mol]: 366.40

Physical Properties

Property code	Value	Unit	Source
gf	-820.76	kJ/mol	Joback Method
hf	-1576.51	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	0.02		Crippen Method
logp	-0.194		Crippen Method
mcvol	267.410	ml/mol	McGowan Method
pc	1393.33	kPa	Joback Method
rinpol	2024.00		NIST Webbook
tb	787.40	K	Joback Method
tc	988.79	K	Joback Method
tf	468.15	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.08	J/mol×K	787.40	Joback Method
cpg	1007.94	J/mol×K	955.22	Joback Method
cpg	993.85	J/mol×K	921.66	Joback Method
cpg	977.74	J/mol×K	888.09	Joback Method
cpg	959.68	J/mol×K	854.53	Joback Method
cpg	939.77	J/mol×K	820.96	Joback Method
cpg	1019.91	J/mol×K	988.79	Joback Method
dvisc	0.0000818	Pa×s	787.40	Joback Method
dvisc	0.0000974	Pa×s	734.19	Joback Method

dvisc	0.0001190	Pa×s	680.98	Joback Method
dvisc	0.0001506	Pa×s	627.78	Joback Method
dvisc	0.0001989	Pa×s	574.57	Joback Method
dvisc	0.0002781	Pa×s	521.36	Joback Method
dvisc	0.0004198	Pa×s	468.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R151278&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

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