

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
rinsol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.08	J/molxK	787.40	Joback Method
cpg	939.77	J/molxK	820.96	Joback Method
cpg	959.68	J/molxK	854.53	Joback Method
cpg	977.74	J/molxK	888.09	Joback Method
cpg	993.85	J/molxK	921.66	Joback Method
cpg	1007.94	J/molxK	955.22	Joback Method
cpg	1019.91	J/molxK	988.79	Joback Method
dvisc	0.0004198	Paxs	468.15	Joback Method
dvisc	0.0002781	Paxs	521.36	Joback Method

dvisc	0.0001989	Paxs	574.57	Joback Method
dvisc	0.0001506	Paxs	627.78	Joback Method
dvisc	0.0001190	Paxs	680.98	Joback Method
dvisc	0.0000974	Paxs	734.19	Joback Method
dvisc	0.0000818	Paxs	787.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R151278&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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