

Xylotriose, permethyl

Inchi:

IVVVORJOYSYZNI-HGKZIHKDSA-N

InchiKey:

C23H42O13

Formula:

COC1COC(OC2COC(OC3COC(OC)C(OC)C3OC)C(OC)C2OC)C(OC)C1OC

SMILES:

526.57

Mol. weight [g/mol]:

Physical Properties

Property code	Value	Unit	Source
gf	-1161.62	kJ/mol	Joback Method
hf	-2256.35	kJ/mol	Joback Method
hfus	76.29	kJ/mol	Joback Method
hvap	102.93	kJ/mol	Joback Method
log10ws	-0.10		Crippen Method
logp	-0.423		Crippen Method
mcvol	378.660	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	2869.00		NIST Webbook
tb	1047.31	K	Joback Method
tc	1282.23	K	Joback Method
tf	634.96	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1481.53	J/mol×K	1047.31	Joback Method
cpg	1475.94	J/mol×K	1243.07	Joback Method
cpg	1487.45	J/mol×K	1203.92	Joback Method
cpg	1493.57	J/mol×K	1164.77	Joback Method
cpg	1494.50	J/mol×K	1125.62	Joback Method
cpg	1490.42	J/mol×K	1086.46	Joback Method
cpg	1458.84	J/mol×K	1282.23	Joback Method
dvisc	0.0000310	Pa×s	1047.31	Joback Method
dvisc	0.0000367	Pa×s	978.58	Joback Method

dvisc	0.0000446	Pa×s	909.86	Joback Method
dvisc	0.0000559	Pa×s	841.13	Joback Method
dvisc	0.0000730	Pa×s	772.41	Joback Method
dvisc	0.0001005	Pa×s	703.69	Joback Method
dvisc	0.0001481	Pa×s	634.96	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R151307&Units=SI

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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