1,2,3,4,5-Penta-O-acetyl-D-xylitol

Other names: Xylitol pentaacetate
xylitol, acetylated
Inchi: InChI=1S/C15H22O10/c1-8(16)21-6-13(23-10(3)18)15(25-12(5)20)14(24-11(4)19)7-22-9
InchiKey: NVKPIAUSOPISJK-UHFFFAOYSA-N
Formula: C15H22O10
SMILES: CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]: 362.33
CAS: 6330-69-4

Physical Properties

Property code	Value	Unit	Source
gf	-1101.50	kJ/mol	Joback Method
hf	-1592.77	kJ/mol	Joback Method
hfus	37.97	kJ/mol	Joback Method
hvap	93.60	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	-0.092		Crippen Method
mcvol	259.410	ml/mol	McGowan Method
pc	1730.34	kPa	Joback Method
rinpol	1837.70		NIST Webbook
rinpol	1837.70		NIST Webbook
tb	922.73	K	Joback Method
tc	1133.29	K	Joback Method
tf	574.61	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.52	J/mol×K	922.73	Joback Method
cpg	821.88	J/mol×K	957.82	Joback Method
cpg	830.79	J/mol×K	992.92	Joback Method
cpg	838.19	J/mol×K	1028.01	Joback Method
cpg	844.04	J/mol×K	1063.10	Joback Method

cpg	848.32	J/mol×K	1098.20	Joback Method
cpg	850.97	J/mol×K	1133.29	Joback Method
dvisc	0.0003285	Pa×s	574.61	Joback Method
dvisc	0.0001826	Pa×s	632.63	Joback Method
dvisc	0.0001121	Pa×s	690.65	Joback Method
dvisc	0.0000742	Pa×s	748.67	Joback Method
dvisc	0.0000521	Pa×s	806.69	Joback Method
dvisc	0.0000384	Pa×s	864.71	Joback Method
dvisc	0.0000294	Pa×s	922.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6330694&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