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

Physical Properties

Property code	Value	Unit	Source
af	0.8633		Cheméo Relay (1.0)
hf	-1911.65	kJ/mol	Cheméo Relay (1.0)
hfus	37.97	kJ/mol	Joback Method
hvap	112.41	kJ/mol	Cheméo Relay (1.0)
ie	9.32	eV	Cheméo Relay (1.0)
log10ws	-0.91		Cheméo Relay (1.0)
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	589.36	K	Cheméo Relay (1.0)
tc	749.48	K	Cheméo Relay (1.0)
tf	330.18	K	Cheméo Relay (1.0)
vc	0.958	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6330694&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie: Ionization energy

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