2,3,5-Tri-O-acetyl-1,4-anhydro-D-xylitol

Other names: 2,3,5-O-triacetyl-1,4-Anhydro-D-xylitol
Inchi: InChI=1S/C11H16O7/c1-6(12)15-4-9-11(18-8(3)14)10(5-16-9)17-7(2)13/h9-11H,4-5H2,1-
InchiKey: AGTSQJAVJCFOSJ-UHFFFAOYSA-N
Formula: C11H16O7
SMILES: CC(=O)OCC1OCC(OC(C)=O)C1OC(C)=O
Mol. weight [g/mol]: 260.24

Physical Properties

Property code	Value	Unit	Source
gf	-725.01	kJ/mol	Joback Method
hf	-1116.97	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	71.70	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	-0.188		Crippen Method
mcvol	183.180	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	1614.75		NIST Webbook
rinpol	1614.75		NIST Webbook
tb	712.84	K	Joback Method
tc	917.89	K	Joback Method
tf	459.20	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.86	J/mol×K	712.84	Joback Method
cpg	550.23	J/mol×K	747.02	Joback Method
cpg	563.65	J/mol×K	781.19	Joback Method
cpg	576.10	J/mol×K	815.37	Joback Method
cpg	587.55	J/mol×K	849.54	Joback Method
cpg	597.98	J/mol×K	883.72	Joback Method
cpg	607.37	J/mol×K	917.89	Joback Method

dvisc	0.0013024	Pa×s	459.20	Joback Method
dvisc	0.0008869	Pa×s	501.47	Joback Method
dvisc	0.0006411	Pa×s	543.75	Joback Method
dvisc	0.0004856	Pa×s	586.02	Joback Method
dvisc	0.0003819	Pa×s	628.29	Joback Method
dvisc	0.0003095	Pa×s	670.57	Joback Method
dvisc	0.0002572	Pa×s	712.84	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=U366029&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