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

Other names: 2,5-O-diAcetyl-1,4-Anhydro-3-O-methyl-D-xylitol
Inchi: InChI=1S/C10H16O6/c1-6(11)14-4-8-10(13-3)9(5-15-8)16-7(2)12/h8-10H,4-5H2,1-3H3
InchiKey: SULWLWFNHXEWRP-UHFFFAOYSA-N
Formula: C10H16O6
SMILES: COC1C(COC(C)=O)OCC1OC(C)=O
Mol. weight [g/mol]: 232.23

Physical Properties

Property code	Value	Unit	Source
gf	-604.51	kJ/mol	Joback Method
hf	-983.75	kJ/mol	Joback Method
hfus	32.47	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-0.14		Crippen Method
logp	-0.105		Crippen Method
mcvol	167.520	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1516.23		NIST Webbook
rinpol	1516.23		NIST Webbook
tb	636.09	K	Joback Method
tc	837.04	K	Joback Method
tf	398.00	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.89	J/mol×K	636.09	Joback Method
cpg	533.18	J/mol×K	803.55	Joback Method
cpg	521.20	J/mol×K	770.06	Joback Method
cpg	508.36	J/mol×K	736.57	Joback Method
cpg	494.68	J/mol×K	703.07	Joback Method
cpg	480.18	J/mol×K	669.58	Joback Method
cpg	544.28	J/mol×K	837.04	Joback Method

dvisc	0.0002719	Pa×s	636.09	Joback Method
dvisc	0.0003266	Pa×s	596.41	Joback Method
dvisc	0.0004027	Pa×s	556.73	Joback Method
dvisc	0.0005128	Pa×s	517.05	Joback Method
dvisc	0.0006797	Pa×s	477.36	Joback Method
dvisc	0.0009483	Pa×s	437.68	Joback Method
dvisc	0.0014137	Pa×s	398.00	Joback Method

Sources

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=U366027&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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