

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

Other names:	2,3-O-diAcetyl-1,4-Anhydro-5-O-methyl-D-xylitol
Inchi:	InChI=1S/C10H16O6/c1-6(11)15-9-5-14-8(4-13-3)10(9)16-7(2)12/h8-10H,4-5H2,1-3H3
InchiKey:	WFFMYHYMXYTKNE-UHFFFAOYSA-N
Formula:	C10H16O6
SMILES:	COCC1OCC(OC(C)=O)C1OC(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	1476.30		NIST Webbook
tb	636.09	K	Joback Method
tc	837.04	K	Joback Method
tf	398.00	K	Joback Method
vc	0.622	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.89	J/molxK	636.09	Joback Method
cpg	480.18	J/molxK	669.58	Joback Method
cpg	494.68	J/molxK	703.07	Joback Method
cpg	508.36	J/molxK	736.57	Joback Method
cpg	521.20	J/molxK	770.06	Joback Method
cpg	533.18	J/molxK	803.55	Joback Method
cpg	544.28	J/molxK	837.04	Joback Method
dvisc	0.0014137	Paxs	398.00	Joback Method

dvisc	0.0009483	Paxs	437.68	Joback Method
dvisc	0.0006797	Paxs	477.36	Joback Method
dvisc	0.0005128	Paxs	517.05	Joback Method
dvisc	0.0004027	Paxs	556.73	Joback Method
dvisc	0.0003266	Paxs	596.41	Joback Method
dvisc	0.0002719	Paxs	636.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U366026&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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