trans-Cyclohexane-1,4-dimethanol, diacetate

Other names:	trans-(4-[(Acetyloxy)methyl]cyclohexyl)methyl acetate
	1,4-Cyclohexanedimethanol, trans, diacetate
	CHDM diacetate derivative, trans isomer
	Trans-1,4-cyclohexanedimethanol, diacetate
Inchi:	InChI=1S/C12H20O4/c1-9(13)15-7-11-3-5-12(6-4-11)8-16-10(2)14/h11-12H,3-8H2,1-2H3
InchiKey:	NNCDHEJIRBOLSS-UHFFFAOYSA-N
Formula:	C12H20O4
SMILES:	CC(=O)OCC1CCC(COC(C)=O)CC1
Mol. weight [g/mol]:	228.28
CAS:	10412-78-9

Physical Properties

Property code	Value	Unit	Source
gf	-400.94	kJ/mol	Joback Method
hf	-746.63	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	60.74	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.919		Crippen Method
mcvol	183.960	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
tb	641.42	K	Joback Method
tc	846.20	K	Joback Method
tf	372.46	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.57	J/mol×K	641.42	Joback Method
cpg	527.23	J/mol×K	675.55	Joback Method
cpg	543.90	J/mol×K	709.68	Joback Method
cpg	559.58	J/mol×K	743.81	Joback Method
cpg	574.26	J/mol×K	777.94	Joback Method

cpg	587.94	J/mol×K	812.07	Joback Method
cpg	600.62	J/mol×K	846.20	Joback Method
dvisc	0.0019188	Pa×s	372.46	Joback Method
dvisc	0.0010612	Pa×s	417.29	Joback Method
dvisc	0.0006584	Pa×s	462.11	Joback Method
dvisc	0.0004445	Pa×s	506.94	Joback Method
dvisc	0.0003198	Pa×s	551.77	Joback Method
dvisc	0.0002418	Pa×s	596.59	Joback Method
dvisc	0.0001901	Pa×s	641.42	Joback Method

Sources

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=C10412789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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