1,2-Cyclopentanediol, diacetate, trans-

Inchi: InChI=1S/C9H14O4/c1-6(10)12-8-4-3-5-9(8)13-7(2)11/h8-9H,3-5H2,1-2H3/t8-,9-/m1/s1
InchiKey: BXAYTJKZGSJCRS-RKDXNWHRSA-N
Formula: C9H14O4
SMILES: CC(=O)OC1CCCC1OC(C)=O
Mol. weight [g/mol]: 186.21
CAS: 26620-22-4

Physical Properties

Property code	Value	Unit	Source
chs	-4661.00	kJ/mol	NIST Webbook
gf	-414.10	kJ/mol	Joback Method
hf	-678.55	kJ/mol	Joback Method
hfus	19.65	kJ/mol	Joback Method
hvap	53.89	kJ/mol	Joback Method
log10ws	-1.43		Crippen Method
logp	1.034		Crippen Method
mcvol	141.690	ml/mol	McGowan Method
pc	2944.08	kPa	Joback Method
tb	568.51	K	Joback Method
tc	776.09	K	Joback Method
tf	342.17	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.51	J/mol×K	568.51	Joback Method
cpg	371.53	J/mol×K	603.11	Joback Method
cpg	385.81	J/mol×K	637.70	Joback Method
cpg	399.32	J/mol×K	672.30	Joback Method
cpg	412.07	J/mol×K	706.90	Joback Method
cpg	424.04	J/mol×K	741.49	Joback Method
cpg	435.24	J/mol×K	776.09	Joback Method
dvisc	0.0019796	Pa×s	342.17	Joback Method

dvisc	0.0012597	Pa×s	379.89	Joback Method
dvisc	0.0008698	Pa×s	417.62	Joback Method
dvisc	0.0006386	Pa×s	455.34	Joback Method
dvisc	0.0004915	Pa×s	493.06	Joback Method
dvisc	0.0003927	Pa×s	530.79	Joback Method
dvisc	0.0003232	Pa×s	568.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26620224&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
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