1,2-Cyclohexanediol diacetate, trans-

Other names: Cyclohexane, 1,2-diacetoxy-, trans-
2-(Acetyloxy)cyclohexyl acetate, (E)-
Inchi: InChI=1S/C10H16O4/c1-7(11)13-9-5-3-4-6-10(9)14-8(2)12/h9-10H,3-6H2,1-2H3/t9-,10-/r
InchiKey: NSTPWRQTPXJRSP-UWVGGRQHSA-N
Formula: C10H16O4
SMILES: CC(=O)OC1CCCCC1OC(C)=O
Mol. weight [g/mol]: 200.23
CAS: 1759-71-3

Physical Properties

Property code	Value	Unit	Source
chs	-5287.30	kJ/mol	NIST Webbook
gf	-417.78	kJ/mol	Joback Method
hf	-705.35	kJ/mol	Joback Method
hfus	20.14	kJ/mol	Joback Method
hvap	56.29	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.424		Crippen Method
mcvol	155.780	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	595.66	K	Joback Method
tc	806.87	K	Joback Method
tf	349.92	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.56	J/mol×K	595.66	Joback Method
cpg	423.19	J/mol×K	630.86	Joback Method
cpg	438.92	J/mol×K	666.06	Joback Method
cpg	453.76	J/mol×K	701.26	Joback Method
cpg	467.69	J/mol×K	736.46	Joback Method
cpg	480.69	J/mol×K	771.67	Joback Method

cpg	492.77	J/mol×K	806.87	Joback Method
dvisc	0.0020866	Pa×s	349.92	Joback Method
dvisc	0.0011937	Pa×s	390.88	Joback Method
dvisc	0.0007592	Pa×s	431.83	Joback Method
dvisc	0.0005222	Pa×s	472.79	Joback Method
dvisc	0.0003813	Pa×s	513.75	Joback Method
dvisc	0.0002916	Pa×s	554.70	Joback Method
dvisc	0.0002314	Pa×s	595.66	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1759713&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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