Acetic acid, 3,4-epoxy-6-methylcyclohexyl methyl ester

Other names: 3,4-Epoxy-6-methylcyclohexylmethyl acetate
4-Methyl-7-oxobicyclo(4.1.0)heptane-3-methanol, acetate
6-Methyl-3,4-epoxycyclohexylmethyl acetate
7-Oxabicyclo(4.1.0)heptane-3-methanol, 4-methyl-, acetate

Inchi: InChI=1S/C10H16O3/c1-6-3-9-10(13-9)4-8(6)5-12-7(2)11/h6,8-10H,3-5H2,1-2H3

InchiKey: OOLNWDDAWUWWTK-UHFFFAOYSA-N

Formula: C10H16O3

SMILES: CC(=O)OCC1CC2OC2CC1C

Mol. weight [g/mol]: 184.23

CAS: 106-85-4

Physical Properties

Property code	Value	Unit	Source
gf	-192.74	kJ/mol	Joback Method
hf	-527.77	kJ/mol	Joback Method
hfus	28.73	kJ/mol	Joback Method
hvap	50.90	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.363		Crippen Method
mcvol	143.350	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
tb	539.85	K	Joback Method
tc	744.00	K	Joback Method
tf	325.07	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.38	J/mol×K	539.85	Joback Method
cpg	391.44	J/mol×K	573.88	Joback Method
cpg	407.56	J/mol×K	607.90	Joback Method
cpg	422.77	J/mol×K	641.93	Joback Method
cpg	437.12	J/mol×K	675.95	Joback Method

cpg	450.63	J/mol×K	709.98	Joback Method
cpg	463.34	J/mol×K	744.00	Joback Method
dvisc	0.0019063	Pa×s	325.07	Joback Method
dvisc	0.0016199	Pa×s	360.87	Joback Method
dvisc	0.0014176	Pa×s	396.66	Joback Method
dvisc	0.0012682	Pa×s	432.46	Joback Method
dvisc	0.0011541	Pa×s	468.26	Joback Method
dvisc	0.0010644	Pa×s	504.05	Joback Method
dvisc	0.0009922	Pa×s	539.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106854&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

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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