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

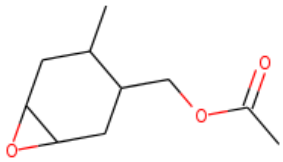
InChI Key: OOLNWDDAWUWWTK-UHFFFAOYSA-N

Formula: C10H16O3

SMILES: CC(=O)OCC1CC2OC2CC1C

Molecular Weight: 184.23

CAS: 106-85-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-192.74	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-527.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	28.73	kJ/mol	Joback Method
$\Delta_{vap} H°$	50.90	kJ/mol	Joback Method
$log P_{oct/wat}$	1.363		Crippen Method
P_c	2707.03	kPa	Joback Method
T_{boil}	539.85	K	Joback Method
T_c	744.00	K	Joback Method
T_{fus}	325.07	K	Joback Method
V_c	0.544	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	374.38	J/mol×K	539.85	Joback Method
η	0.0009916	Pa×s	539.85	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/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
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).