

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/h6,8-10
H,3-5H2,1-2H3

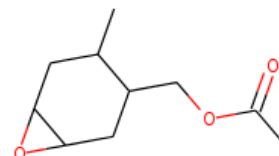
InChI Key: OOLNWDDAWUWWTk-UHFFFAOYSA-N

Formula: C10H16O3

SMILES: CC(=O)OCC1CC2OC2CC1C

Molecular Weight: 184.23

CAS: 106-85-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-192.74	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-527.77	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	28.73	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	50.90	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	374.38	J/mol×K	539.85	Joback Method
η	0.0009916	Paxs	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](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/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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