Levo-menthoxyacetic acid

Other names: (-)-Menthoxyacetic acid; (-)-Menthyloxyacetic acid; Acetic acid, [[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]-, [1R-(1«alpha»,2«beta»,5«alpha»)]-; L-Menthoxyacetic acid; L-p-menth-3-yloxyacetic acid.

InChI: InChI=1S/C12H22O3/c1-8(2)10-5-4-9(3)6-11(10)15-7-12(13)14/h8-11H,4-7H2,1-3H3,(H,13,14)

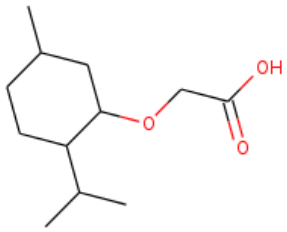
InChI Key: CILPHQCEVYJUDN-UHFFFAOYSA-N

Formula: C12H22O3

SMILES: CC(C)C1CCC(C)CC1OCC(=O)O

Molecular Weight: 214.30

CAS: 40248-63-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-313.99	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-679.68	kJ/mol	Joback Method
$\Delta_{fus} H°$	24.16	kJ/mol	Joback Method
$\Delta_{vap} H°$	67.56	kJ/mol	Joback Method
$logP_{oct/wat}$	2.55		Crippen Method
P_c	2300.32	kPa	Joback Method
T_{boil}	436.70	K	NIST Webbook
T_c	843.77	K	Joback Method
T_{fus}	341.88	K	Joback Method
V_c	0.68	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	526.75	J/mol×K	652.2	Joback Method
η	0.00	Pa×s	652.2	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H22O3/c1-8(2)10-5-4-9(3)6-11(10)15-7-12(13)14/h8-11H,4-7H2,1-3H3,(H,13,14)
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).