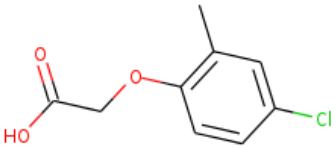
[(4-Chloro-o-tolyl)oxy]acetic acid



Other names: (2-Methyl-4-chlorophenoxy)acetic acid; (4-Chloro-2-methylphenoxy)acetic acid; (4-Chloro-o-cresoxy)acetic acid; (4-Chloro-o-toloxy)acetic acid; 2,4-MCPA; 2-(4-Chloro-2-methylphenoxy)acetic acid; 2-Methyl-4-chlorphenoxyessigsaeure; 2M-4C; 2M-4Ch; 2M-4Kh; 4K-2M; Acetic acid, (4-chloro-2-methylphenoxy)-; Acetic acid, (4-chloro-o-toloxy)-; Acetic acid, 2-(4-chloro-2-methylphenoxy)-; Acetic acid, [(4-chloro-o-tolyl)oxy]-; Acme MCPA amine 4; Agricorn 500 II; Agritox; Agritox 50; Agroxon; Agroxone; Albar-M; Anicon M; Anicon kombi; Atlas MCPA; B-Selektonon M; BH MCPA; Bordermaster; Brominal M & plus; Campbell's MCPA 25, 50; Cekherbex; Chiptox; Chwastox 30; Cornox-M; Dicopur-M; Dicotex; Dikotes; Dikotex; Dow MCP amine weed killer; Emcepan; Empal; Hedapur M 52; Hedarex M; Hedonal M; Herbicide M; Hormoneste; Hormotuho; Hornotuho; Kilsem; Kilsem4k-2m; Krezone; Kwas 4-chloro-2-metylofenoksyoctowy; Kyselina 4-chlor-2-methylfenoxyoctova; Legumex DB; Leuna M; Leyspray; Linormone; M 40; MCP; MCPA; Mecaphar; Mephanac; Metaxon; Methoxone; Methyl chlorophenoxy acetic acid; Netazol; Okultin M; Phenoxylene 50; Phenoxylene plus; Phenoxylene super; Raphone; Razol dock killer; Rhomenc; Rhomene; Rhonox; Selektonon M; Seppic MMD; Shamrox; Soviet technical herbicide 2M-4C; Trasan; U 46 M-FLUID; Ustinex; Vacate; Verdone; Vesakontuho MCPA; Weed-rhap; Weedar MCPA; Weedar mcpa concentrate; Weedone mcpa ester; Zelan.

InChI: InChI=1S/C9H9ClO3/c1-6-4-7(10)2-3-8(6)13-5-9(11)12/h2-4H,5H2,1H3,(H,11,12)

InChI Key: WHKUVVPPKQRRBV-UHFFFAOYSA-N

Formula: C9H9ClO3

SMILES: Cc1cc(Cl)ccc1OCC(=O)O

Molecular Weight: 200.62

CAS: 94-74-6

Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-264.62	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-428.27	kJ/mol	Joback Method
$\Delta_{fus} H°$	23.40	kJ/mol	Joback Method
$\Delta_{vap} H°$	69.45	kJ/mol	Joback Method
$logP_{oct/wat}$	2.11		Crippen Method
P_c	3543.08	kPa	Joback Method
T_{boil}	647.86	K	Joback Method

Property	Value	Unit	Source
T_c	854.75	K	Joback Method
T_{fus}	393.44 ± 0.20	K	NIST Webbook
T_{fus}	392.70 ± 0.20	K	NIST Webbook
V_c	0.52	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	323.99	J/mol×K	647.86	Joback Method
η	0.00	Pa×s	647.86	Joback Method
$\Delta_{fus}H$	29.98	kJ/mol	392.9	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C9H9ClO3/c1-6-4-7(10)2-3-8(6)13-5-9(11)12/h2-4H,5H2,1H3,(H,11,12)
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).
$\Delta_{fus}\mathbf{H}$: Enthalpy of fusion at a given temperature (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).