

[(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-toloxo)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-toloxo)-
- 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-Selektionon 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
Hormotuhu
Hornotuhu
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
Phenoxylyene 50
Phenoxylyene plus
Phenoxylyene 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)
InchiKey: WHKUVVPPKQRRBV-UHFFFAOYSA-N
Formula: C9H9ClO3
SMILES: Cc1cc(Cl)ccc1OCC(=O)O
Mol. weight [g/mol]: 200.62
CAS: 94-74-6

Physical Properties

Property code	Value	Unit	Source
gf	-264.62	kJ/mol	Joback Method
hf	-428.27	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Joback Method
hvap	69.45	kJ/mol	Joback Method
log10ws	-2.23		Aqueous Solubility Prediction Method
logp	2.112		Crippen Method
mcvol	139.460	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
tb	647.86	K	Joback Method
tc	854.75	K	Joback Method
tf	393.44 ± 0.20	K	NIST Webbook
tf	392.70 ± 0.20	K	NIST Webbook
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.99	J/molxK	647.86	Joback Method
cpg	333.23	J/molxK	682.34	Joback Method
cpg	341.92	J/molxK	716.82	Joback Method

cpg	350.07	J/mol×K	751.31	Joback Method
cpg	357.70	J/mol×K	785.79	Joback Method
cpg	364.79	J/mol×K	820.27	Joback Method
cpg	371.37	J/mol×K	854.75	Joback Method
dvisc	0.0014442	Paxs	405.55	Joback Method
dvisc	0.0006838	Paxs	445.94	Joback Method
dvisc	0.0003666	Paxs	486.32	Joback Method
dvisc	0.0002162	Paxs	526.71	Joback Method
dvisc	0.0001375	Paxs	567.09	Joback Method
dvisc	0.0000929	Paxs	607.48	Joback Method
dvisc	0.0000659	Paxs	647.86	Joback Method
hfust	29.98	kJ/mol	392.90	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C94746&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
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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