Butanoic acid, 4-(4-chloro-2-methylphenoxy)-

Other names:	Butyric acid, 4-[(4-chloro-o-tolyl)oxy]-
	«gamma»-MCPB
	(2-Methyl-4-Chlorophenoxy)butyric acid
	(4-Chloro-2-methylphenoxy)butyric acid
	[(4-Chloro-o-tolyl)oxy]butyric acid
	Bexone
	MCPB
	Thitrol
	Trifolex
	U46 MCPB
	2,4-MCPB
	2M 4KhM
	2M-4XM
	4-(2-Methyl-4-Chlorophenoxy)butyric acid
	4-(4-Chloro-2-methylphenoxy)butanoic acid
	4-(4-Chloro-2-methylphenoxy)butyric acid
	4MCPB
	4-(4-Chloro-o-tolyloxy)butyric acid
	«gamma»-(2-Methyl-4-chlorophenoxy)butyric acid
	«gamma»-(4-Chloro-2-methylphenoxy)butyric acid
	Bexane
	Legumex
	MCP-Butyric
	PDQ
	Tritrol
	Trotox
	4-(4-Chlor-2-methyl-phenoxy)-buttersaeure
	Kyselina 4-(4-chlor-2-methylfenoxy)maselna
	MB 3046
	4-(2-Methyl-4-chlorphenoxy)-buttersaeure
	Belmac straight
	Fisons 18-15, MCPB
	NSC 102796
Inchi:	InChI=1S/C11H13ClO3/c1-8-7-9(12)4-5-10(8)15-6-2-3-11(13)14/h4-5,7H,2-3,6H2,1H3,(H
InchiKey:	LLWADFLAOKUBDR-UHFFFAOYSA-N
Formula:	C10H13ClO3
SMILES:	Cc1cc(Cl)ccc1OCCCC(=O)O
Mol. weight [g/mol]:	216.66
CAS:	94-81-5

Physical Properties

Property code	Value	Unit	Source
gf	-247.78	kJ/mol	Joback Method
hf	-469.55	kJ/mol	Joback Method
hfus	28.58	kJ/mol	Joback Method
hvap	73.90	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.892		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1820.00		NIST Webbook
tb	693.62	K	Joback Method
tc	895.15	K	Joback Method
tf	428.09	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.70	J/mol×K	693.62	Joback Method
cpg	432.40	J/mol×K	727.21	Joback Method
cpg	442.46	J/mol×K	760.80	Joback Method
cpg	451.90	J/mol×K	794.39	Joback Method
cpg	460.72	J/mol×K	827.97	Joback Method
cpg	468.94	J/mol×K	861.56	Joback Method
cpg	476.57	J/mol×K	895.15	Joback Method
dvisc	0.0011115	Pa×s	428.09	Joback Method
dvisc	0.0005126	Pa×s	472.34	Joback Method
dvisc	0.0002699	Pa×s	516.60	Joback Method
dvisc	0.0001573	Pa×s	560.86	Joback Method
dvisc	0.0000992	Pa×s	605.11	Joback Method
dvisc	0.0000666	Pa×s	649.37	Joback Method
dvisc	0.0000470	Pa×s	693.62	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C94815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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