Mecoprop methyl ester

Other names:	MCPP ester
	Propanoic acid, 2-(2-methyl-4-chlorophenyloxy)-, methyl ester
	CMPP methyl ester
	MCPP methyl ester
	Mecoprop-Methyl
	Propanoic acid, 2-(4-chloro-2-methylphenoxy), methyl ester
	Methyl 2-(4-chloro-2-methylphenoxy)propanoate
Inchi:	InChI=1S/C11H13ClO3/c1-7-6-9(12)4-5-10(7)15-8(2)11(13)14-3/h4-6,8H,1-3H3
InchiKey:	YWGAULPFWIQKRB-UHFFFAOYSA-N
Formula:	C11H13ClO3
SMILES:	COC(=O)C(C)Oc1ccc(Cl)cc1C
Mol. weight [g/mol]:	228.67
CAS:	23844-56-6

Physical Properties

Property code	Value	Unit	Source
gf	-218.40	kJ/mol	Joback Method
hf	-454.82	kJ/mol	Joback Method
hfus	22.16	kJ/mol	Joback Method
hvap	59.24	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.589		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1519.00		NIST Webbook
rinpol	1514.00		NIST Webbook
ripol	2115.00		NIST Webbook
ripol	2115.00		NIST Webbook
tb	623.42	K	Joback Method
tc	840.62	K	Joback Method
tf	374.50	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.79	J/mol×K	623.42	Joback Method
cpg	455.26	J/mol×K	804.42	Joback Method
cpg	445.07	J/mol×K	768.22	Joback Method
cpg	434.12	J/mol×K	732.02	Joback Method
cpg	422.42	J/mol×K	695.82	Joback Method
cpg	409.98	J/mol×K	659.62	Joback Method
cpg	464.69	J/mol×K	840.62	Joback Method
dvisc	0.0001398	Pa×s	623.42	Joback Method
dvisc	0.0001753	Pa×s	581.93	Joback Method
dvisc	0.0002275	Pa×s	540.45	Joback Method
dvisc	0.0003084	Pa×s	498.96	Joback Method
dvisc	0.0004417	Pa×s	457.47	Joback Method
dvisc	0.0006796	Pa×s	415.99	Joback Method
dvisc	0.0011503	Pa×s	374.50	Joback Method

Sources

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=C23844566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume