Mcpb methyl ester

Other names: Butanoic acid, 4-(2-methyl-4-chlorophenoxy)-, methyl ester
Inchi: InChI=1S/C12H15ClO3/c1-9-8-10(13)5-6-11(9)16-7-3-4-12(14)15-2/h5-6,8H,3-4,7H2,1-2
InchiKey: FWDQLSHRVKQKBS-UHFFFAOYSA-N
Formula: C12H15ClO3
SMILES: COC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]: 242.70
CAS: 57153-18-1

Physical Properties

Property code	Value	Unit	Source
gf	-207.54	kJ/mol	Joback Method
hf	-470.18	kJ/mol	Joback Method
hfus	28.27	kJ/mol	Joback Method
hvap	61.86	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	2.980		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1753.00		NIST Webbook
ripol	2421.00		NIST Webbook
ripol	2420.00		NIST Webbook
ripol	2420.00		NIST Webbook
tb	646.74	K	Joback Method
tc	856.27	K	Joback Method
tf	400.77	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.69	J/mol×K	646.74	Joback Method

cpg	459.28	J/mol×K	681.66	Joback Method
cpg	472.10	J/mol×K	716.58	Joback Method
cpg	484.17	J/mol×K	751.50	Joback Method
cpg	495.48	J/mol×K	786.42	Joback Method
cpg	506.03	J/mol×K	821.35	Joback Method
cpg	515.82	J/mol×K	856.27	Joback Method
dvisc	0.0009316	Pa×s	400.77	Joback Method
dvisc	0.0005819	Pa×s	441.76	Joback Method
dvisc	0.0003936	Pa×s	482.76	Joback Method
dvisc	0.0002831	Pa×s	523.75	Joback Method
dvisc	0.0002136	Pa×s	564.75	Joback Method
dvisc	0.0001674	Pa×s	605.75	Joback Method
dvisc	0.0001353	Pa×s	646.74	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=C57153181&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume