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

Physical Properties

Property code	Value	Unit	Source
hfus	28.27	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-3.53		Cheméo Relay (1.0)
logp	2.980		Crippen Method
mcvol	181.730	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1729.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1729.00		NIST Webbook
ripol	2421.00		NIST Webbook
ripol	2420.00		NIST Webbook
ripol	2420.00		NIST Webbook
tb	575.93	K	Cheméo Relay (1.0)
tf	300.59	K	Cheméo Relay (1.0)

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	441.77	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57153181&Units=SI

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

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

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
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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
tf: Normal melting (fusion) point