Acetic acid, (4-chloro-2-methylphenoxy)-, ethyl ester

Other names: Acetic acid, ((4-chloro-o-tolyl)oxy)-, ethyl ester
Ethyl 2-methyl-4-chlorophenoxyacetate
Mcpa ethyl ester
Mcpee
MCPA-ethyl
4-Chloro-2-methylphenoxyacetic acid ethyl ester
2M-4C, ethyl ester
ethyl 4-chloro-o-tolyloxyacetate

Inchi: InChI=1S/C11H13ClO3/c1-3-14-11(13)7-15-10-5-4-9(12)6-8(10)2/h4-6H,3,7H2,1-2H3

InchiKey: OUYDEKFRLSFDMU-UHFFFAOYSA-N

Formula: C11H13ClO3

SMILES: CCOC(=O)COc1ccc(Cl)cc1C

Mol. weight [g/mol]: 228.67

CAS: 2698-38-6

Physical Properties

Property code	Value	Unit	Source
gf	-215.96	kJ/mol	Joback Method
hf	-449.54	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.590		Crippen Method
mcvol	167.640	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1635.00		NIST Webbook
tb	623.86	K	Joback Method
tc	836.76	K	Joback Method
tf	389.50	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.31	J/mol×K	623.86	Joback Method
cpg	409.19	J/mol×K	659.34	Joback Method
cpg	421.37	J/mol×K	694.83	Joback Method
cpg	432.85	J/mol×K	730.31	Joback Method
cpg	443.61	J/mol×K	765.79	Joback Method
cpg	453.65	J/mol×K	801.27	Joback Method
cpg	462.98	J/mol×K	836.76	Joback Method
dvisc	0.0009740	Pa×s	389.50	Joback Method
dvisc	0.0006188	Pa×s	428.56	Joback Method
dvisc	0.0004241	Pa×s	467.62	Joback Method
dvisc	0.0003081	Pa×s	506.68	Joback Method
dvisc	0.0002343	Pa×s	545.74	Joback Method
dvisc	0.0001848	Pa×s	584.80	Joback Method
dvisc	0.0001501	Pa×s	623.86	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=C2698386&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume