4-(4-Chloro-2-methylphenoxy)butyric acid, propyl ester

Inchi: InChI=1S/C14H19ClO3/c1-3-8-18-14(16)5-4-9-17-13-7-6-12(15)10-11(13)2/h6-7,10H,3-5

InchiKey: PXDSUQMRJGJUHZ-UHFFFAOYSA-N

Formula: C14H19ClO3

SMILES: CCCOC(=O)CCCOc1ccc(Cl)cc1C

Mol. weight [g/mol]: 270.75

Physical Properties

Property code	Value	Unit	Source
gf	-190.70	kJ/mol	Joback Method
hf	-511.46	kJ/mol	Joback Method
hfus	33.45	kJ/mol	Joback Method
hvap	66.31	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.761		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tb	692.50	K	Joback Method
tc	896.30	K	Joback Method
tf	423.31	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.82	J/mol×K	692.50	Joback Method
cpg	613.83	J/mol×K	862.33	Joback Method
cpg	602.50	J/mol×K	828.37	Joback Method
cpg	590.35	J/mol×K	794.40	Joback Method
cpg	577.35	J/mol×K	760.43	Joback Method
cpg	563.51	J/mol×K	726.47	Joback Method
cpg	624.32	J/mol×K	896.30	Joback Method
dvisc	0.0001081	Pa×s	692.50	Joback Method

dvisc	0.0001350	Pa×s	647.63	Joback Method
dvisc	0.0001743	Pa×s	602.77	Joback Method
dvisc	0.0002344	Pa×s	557.90	Joback Method
dvisc	0.0003321	Pa×s	513.04	Joback Method
dvisc	0.0005028	Pa×s	468.18	Joback Method
dvisc	0.0008314	Pa×s	423.31	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U415077&Units=SI

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