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

Inchi: InChI=1S/C16H23ClO3/c1-3-4-5-10-20-16(18)7-6-11-19-15-9-8-14(17)12-13(15)2/h8-9,1
InchiKey: LAMDMGFZZQRCSZ-UHFFFAOYSA-N
Formula: C16H23ClO3
SMILES: CCCCCOC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]: 298.81

Physical Properties

Property code	Value	Unit	Source
gf	-173.86	kJ/mol	Joback Method
hf	-552.74	kJ/mol	Joback Method
hfus	38.63	kJ/mol	Joback Method
hvap	70.76	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.541		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	738.26	K	Joback Method
tc	937.97	K	Joback Method
tf	445.85	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.14	J/mol×K	738.26	Joback Method
cpg	672.63	J/mol×K	771.54	Joback Method
cpg	687.20	J/mol×K	804.83	Joback Method
cpg	700.85	J/mol×K	838.11	Joback Method
cpg	713.59	J/mol×K	871.40	Joback Method
cpg	725.43	J/mol×K	904.68	Joback Method
cpg	736.38	J/mol×K	937.97	Joback Method
dvisc	0.0007211	Pa×s	445.85	Joback Method

dvisc	0.0004234	Pa×s	494.59	Joback Method
dvisc	0.0002735	Pa×s	543.32	Joback Method
dvisc	0.0001898	Pa×s	592.06	Joback Method
dvisc	0.0001393	Pa×s	640.79	Joback Method
dvisc	0.0001068	Pa×s	689.52	Joback Method
dvisc	0.0000848	Pa×s	738.26	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=U415080&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