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

Inchi: InChI=1S/C17H25ClO3/c1-13(2)6-4-11-21-17(19)7-5-10-20-16-9-8-15(18)12-14(16)3/h8-

InchiKey: ASXVPVAGPZBYHS-UHFFFAOYSA-N

Formula: C17H25ClO3

SMILES: Cc1cc(Cl)ccc1OCCCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 312.83

Physical Properties

Property code	Value	Unit	Source
gf	-167.88	kJ/mol	Joback Method
hf	-578.66	kJ/mol	Joback Method
hfus	37.70	kJ/mol	Joback Method
hvap	72.60	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.787		Crippen Method
mcvol	252.180	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	760.70	K	Joback Method
tc	961.76	K	Joback Method
tf	442.12	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.55	J/mol×K	760.70	Joback Method
cpg	729.59	J/mol×K	794.21	Joback Method
cpg	744.63	J/mol×K	827.72	Joback Method
cpg	758.67	J/mol×K	861.23	Joback Method
cpg	771.74	J/mol×K	894.74	Joback Method
cpg	783.85	J/mol×K	928.25	Joback Method
cpg	795.01	J/mol×K	961.76	Joback Method
dvisc	0.0007634	Pa×s	442.12	Joback Method

dvisc	0.0004122	Pa×s	495.22	Joback Method
dvisc	0.0002507	Pa×s	548.31	Joback Method
dvisc	0.0001665	Pa×s	601.41	Joback Method
dvisc	0.0001182	Pa×s	654.51	Joback Method
dvisc	0.0000883	Pa×s	707.60	Joback Method
dvisc	0.0000687	Pa×s	760.70	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=U415081&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume