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

Inchi: InChI=1S/C19H29ClO3/c1-3-4-5-6-7-8-13-23-19(21)10-9-14-22-18-12-11-17(20)15-16(18
InchiKey: WROBQVBWQOGTTQ-UHFFFAOYSA-N
Formula: C19H29ClO3
SMILES: CCCCCCCCOC(=O)CCCOc1ccc(Cl)cc1C
Mol. weight [g/mol]: 340.88

Physical Properties

Property code	Value	Unit	Source
gf	-148.60	kJ/mol	Joback Method
hf	-614.66	kJ/mol	Joback Method
hfus	46.40	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	5.711		Crippen Method
mcvol	280.360	ml/mol	McGowan Method
pc	1323.28	kPa	Joback Method
rinpol	3000.00		NIST Webbook
rinpol	3000.00		NIST Webbook
tb	806.90	K	Joback Method
tc	1004.33	K	Joback Method
tf	479.66	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.81	J/mol×K	806.90	Joback Method
cpg	899.36	J/mol×K	971.43	Joback Method
cpg	887.07	J/mol×K	938.52	Joback Method
cpg	873.79	J/mol×K	905.62	Joback Method
cpg	859.50	J/mol×K	872.71	Joback Method
cpg	844.18	J/mol×K	839.81	Joback Method
cpg	910.67	J/mol×K	1004.33	Joback Method
dvisc	0.0000572	Pa×s	806.90	Joback Method

dvisc	0.0000729	Pa×s	752.36	Joback Method
dvisc	0.0000964	Pa×s	697.82	Joback Method
dvisc	0.0001338	Pa×s	643.28	Joback Method
dvisc	0.0001971	Pa×s	588.74	Joback Method
dvisc	0.0003144	Pa×s	534.20	Joback Method
dvisc	0.0005575	Pa×s	479.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415084&Units=SI
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

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