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

Inchi: InChI=1S/C29H49ClO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-33-29(31)20-19

InchiKey: LTWFHUCTTCKZOK-UHFFFAOYSA-N

Formula: C29H49ClO3

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

Mol. weight [g/mol]: 481.15

Physical Properties

Property code	Value	Unit	Source
gf	-64.40	kJ/mol	Joback Method
hf	-821.06	kJ/mol	Joback Method
hfus	72.30	kJ/mol	Joback Method
hvap	99.70	kJ/mol	Joback Method
log10ws	-10.41		Crippen Method
logp	9.612		Crippen Method
mcvol	421.260	ml/mol	McGowan Method
pc	726.92	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	1035.70	K	Joback Method
tc	1276.38	K	Joback Method
tf	592.36	K	Joback Method
vc	1.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1444.06	J/mol×K	1035.70	Joback Method
cpg	1463.46	J/mol×K	1075.81	Joback Method
cpg	1480.97	J/mol×K	1115.93	Joback Method
cpg	1496.68	J/mol×K	1156.04	Joback Method
cpg	1510.66	J/mol×K	1196.16	Joback Method
cpg	1522.99	J/mol×K	1236.27	Joback Method
cpg	1533.75	J/mol×K	1276.38	Joback Method
dvisc	0.0001813	Pa×s	592.36	Joback Method

dvisc	0.0000918	Pa×s	666.25	Joback Method
dvisc	0.0000533	Pa×s	740.14	Joback Method
dvisc	0.0000341	Pa×s	814.03	Joback Method
dvisc	0.0000235	Pa×s	887.92	Joback Method
dvisc	0.0000172	Pa×s	961.81	Joback Method
dvisc	0.0000131	Pa×s	1035.70	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=U415094&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