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

Inchi: InChI=1S/C27H45ClO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-21-31-27(29)18-17-22-30

InchiKey: ABLFLNJSKJOBCU-UHFFFAOYSA-N

Formula: C27H45ClO3

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

Mol. weight [g/mol]: 453.10

Physical Properties

Property code	Value	Unit	Source
gf	-81.24	kJ/mol	Joback Method
hf	-779.78	kJ/mol	Joback Method
hfus	67.12	kJ/mol	Joback Method
hvap	95.25	kJ/mol	Joback Method
log10ws	-9.57		Crippen Method
logp	8.832		Crippen Method
mcvol	393.080	ml/mol	McGowan Method
pc	808.45	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	989.94	K	Joback Method
tc	1213.84	K	Joback Method
tf	569.82	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1316.80	J/mol×K	989.94	Joback Method
cpg	1335.38	J/mol×K	1027.26	Joback Method
cpg	1352.36	J/mol×K	1064.57	Joback Method
cpg	1367.77	J/mol×K	1101.89	Joback Method
cpg	1381.69	J/mol×K	1139.20	Joback Method
cpg	1394.15	J/mol×K	1176.52	Joback Method
cpg	1405.23	J/mol×K	1213.84	Joback Method
dvisc	0.0002328	Pa×s	569.82	Joback Method

dvisc	0.0001201	Pa×s	639.84	Joback Method
dvisc	0.0000706	Pa×s	709.86	Joback Method
dvisc	0.0000457	Pa×s	779.88	Joback Method
dvisc	0.0000317	Pa×s	849.90	Joback Method
dvisc	0.0000233	Pa×s	919.92	Joback Method
dvisc	0.0000179	Pa×s	989.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415092&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

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