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

Inchi: InChI=1S/C25H41ClO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-29-25(27)16-15-20-28-24-18

InchiKey: QHNPDYQMPIWYKA-UHFFFAOYSA-N

Formula: C25H41ClO3

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

Mol. weight [g/mol]: 425.04

Physical Properties

Property code	Value	Unit	Source
gf	-98.08	kJ/mol	Joback Method
hf	-738.50	kJ/mol	Joback Method
hfus	61.94	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-8.73		Crippen Method
logp	8.052		Crippen Method
mcvol	364.900	ml/mol	McGowan Method
pc	904.52	kPa	Joback Method
rinpol	1721.00		NIST Webbook
rinpol	1721.00		NIST Webbook
tb	944.18	K	Joback Method
tc	1155.95	K	Joback Method
tf	547.28	K	Joback Method
vc	1.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.11	J/mol×K	944.18	Joback Method
cpg	1209.02	J/mol×K	979.47	Joback Method
cpg	1225.52	J/mol×K	1014.77	Joback Method
cpg	1240.66	J/mol×K	1050.06	Joback Method
cpg	1254.47	J/mol×K	1085.36	Joback Method
cpg	1266.99	J/mol×K	1120.65	Joback Method
cpg	1278.26	J/mol×K	1155.95	Joback Method
dvisc	0.0002956	Pa×s	547.28	Joback Method

dvisc	0.0001556	Pa×s	613.43	Joback Method
dvisc	0.0000928	Pa×s	679.58	Joback Method
dvisc	0.0000607	Pa×s	745.73	Joback Method
dvisc	0.0000425	Pa×s	811.88	Joback Method
dvisc	0.0000314	Pa×s	878.03	Joback Method
dvisc	0.0000242	Pa×s	944.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415090&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