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

Inchi: InChI=1S/C24H39ClO3/c1-3-4-5-6-7-8-9-10-11-12-13-18-28-24(26)15-14-19-27-23-17-16

InchiKey: YNFWZKLRUMOIHX-UHFFFAOYSA-N

Formula: C24H39ClO3

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

Mol. weight [g/mol]: 411.02

Physical Properties

Property code	Value	Unit	Source
gf	-106.50	kJ/mol	Joback Method
hf	-717.86	kJ/mol	Joback Method
hfus	59.35	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.662		Crippen Method
mcvol	350.810	ml/mol	McGowan Method
pc	959.10	kPa	Joback Method
rinpol	3527.00		NIST Webbook
rinpol	3527.00		NIST Webbook
tb	921.30	K	Joback Method
tc	1128.55	K	Joback Method
tf	536.01	K	Joback Method
vc	1.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1128.98	J/mol×K	921.30	Joback Method
cpg	1204.16	J/mol×K	1094.01	Joback Method
cpg	1191.64	J/mol×K	1059.47	Joback Method
cpg	1177.89	J/mol×K	1024.93	Joback Method
cpg	1162.89	J/mol×K	990.38	Joback Method
cpg	1146.60	J/mol×K	955.84	Joback Method
cpg	1215.50	J/mol×K	1128.55	Joback Method
dvisc	0.0000281	Pa×s	921.30	Joback Method

dvisc	0.0000364	Pa×s	857.08	Joback Method
dvisc	0.0000490	Pa×s	792.87	Joback Method
dvisc	0.0000697	Pa×s	728.65	Joback Method
dvisc	0.0001060	Pa×s	664.44	Joback Method
dvisc	0.0001764	Pa×s	600.23	Joback Method
dvisc	0.0003316	Pa×s	536.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415089&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

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