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

Inchi: InChI=1S/C22H35ClO3/c1-3-4-5-6-7-8-9-10-11-16-26-22(24)13-12-17-25-21-15-14-20(23

InchiKey: ZKACEPCRHZMOBP-UHFFFAOYSA-N

Formula: C22H35ClO3

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

Mol. weight [g/mol]: 382.96

Physical Properties

Property code	Value	Unit	Source
gf	-123.34	kJ/mol	Joback Method
hf	-676.58	kJ/mol	Joback Method
hfus	54.17	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.881		Crippen Method
mcvol	322.630	ml/mol	McGowan Method
pc	1084.20	kPa	Joback Method
rinpol	3320.00		NIST Webbook
rinpol	3320.00		NIST Webbook
tb	875.54	K	Joback Method
tc	1076.49	K	Joback Method
tf	513.47	K	Joback Method
vc	1.250	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1006.43	J/mol×K	875.54	Joback Method
cpg	1080.24	J/mol×K	1043.00	Joback Method
cpg	1067.76	J/mol×K	1009.51	Joback Method
cpg	1054.16	J/mol×K	976.02	Joback Method
cpg	1039.43	J/mol×K	942.52	Joback Method
cpg	1023.52	J/mol×K	909.03	Joback Method
cpg	1091.64	J/mol×K	1076.49	Joback Method
dvisc	0.0000376	Pa×s	875.54	Joback Method

dvisc	0.0000484	Pa×s	815.19	Joback Method
dvisc	0.0000648	Pa×s	754.85	Joback Method
dvisc	0.0000912	Pa×s	694.50	Joback Method
dvisc	0.0001371	Pa×s	634.16	Joback Method
dvisc	0.0002246	Pa×s	573.82	Joback Method
dvisc	0.0004130	Pa×s	513.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415087&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