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

Inchi: InChI=1S/C21H33ClO3/c1-3-4-5-6-7-8-9-10-15-25-21(23)12-11-16-24-20-14-13-19(22)17

InchiKey: NYSMPKZWYRLOIP-UHFFFAOYSA-N

Formula: C21H33ClO3

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

Mol. weight [g/mol]: 368.94

Physical Properties

Property code	Value	Unit	Source
gf	-131.76	kJ/mol	Joback Method
hf	-655.94	kJ/mol	Joback Method
hfus	51.58	kJ/mol	Joback Method
hvap	81.89	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.491		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
pc	1156.14	kPa	Joback Method
rinpol	3216.00		NIST Webbook
rinpol	3216.00		NIST Webbook
tb	852.66	K	Joback Method
tc	1051.71	K	Joback Method
tf	502.20	K	Joback Method
vc	1.194	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	946.13	J/mol×K	852.66	Joback Method
cpg	962.98	J/mol×K	885.83	Joback Method
cpg	978.69	J/mol×K	919.01	Joback Method
cpg	993.29	J/mol×K	952.18	Joback Method
cpg	1006.80	J/mol×K	985.36	Joback Method
cpg	1019.24	J/mol×K	1018.53	Joback Method
cpg	1030.63	J/mol×K	1051.71	Joback Method
dvisc	0.0004584	Pa×s	502.20	Joback Method

dvisc	0.0002522	Pa×s	560.61	Joback Method
dvisc	0.0001553	Pa×s	619.02	Joback Method
dvisc	0.0001040	Pa×s	677.43	Joback Method
dvisc	0.0000742	Pa×s	735.84	Joback Method
dvisc	0.0000556	Pa×s	794.25	Joback Method
dvisc	0.0000434	Pa×s	852.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415086&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