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

Inchi: InChI=1S/C18H27ClO3/c1-3-4-5-6-7-12-22-18(20)9-8-13-21-17-11-10-16(19)14-15(17)2/

InchiKey: ACRHGCFXTOOYHZ-UHFFFAOYSA-N

Formula: C18H27ClO3

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

Mol. weight [g/mol]: 326.86

Physical Properties

Property code	Value	Unit	Source
gf	-157.02	kJ/mol	Joback Method
hf	-594.02	kJ/mol	Joback Method
hfus	43.81	kJ/mol	Joback Method
hvap	75.21	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.321		Crippen Method
mcvol	266.270	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2895.00		NIST Webbook
tb	784.02	K	Joback Method
tc	981.63	K	Joback Method
tf	468.39	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.94	J/mol×K	784.02	Joback Method
cpg	840.56	J/mol×K	948.70	Joback Method
cpg	828.39	J/mol×K	915.76	Joback Method
cpg	815.25	J/mol×K	882.83	Joback Method
cpg	801.14	J/mol×K	849.89	Joback Method
cpg	786.04	J/mol×K	816.96	Joback Method
cpg	851.79	J/mol×K	981.63	Joback Method
dvisc	0.0000655	Pa×s	784.02	Joback Method
dvisc	0.0000831	Pa×s	731.41	Joback Method

dvisc	0.0001094	Pa×s	678.81	Joback Method
dvisc	0.0001509	Pa×s	626.20	Joback Method
dvisc	0.0002208	Pa×s	573.60	Joback Method
dvisc	0.0003488	Pa×s	521.00	Joback Method
dvisc	0.0006106	Pa×s	468.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415083&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