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

Inchi: InChI=1S/C15H21ClO3/c1-11(2)10-19-15(17)5-4-8-18-14-7-6-13(16)9-12(14)3/h6-7,9,11
InchiKey: YWYRKYNYHRGXSR-UHFFFAOYSA-N
Formula: C15H21ClO3
SMILES: Cc1cc(Cl)ccc1OCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 284.78

Physical Properties

Property code	Value	Unit	Source
gf	-184.72	kJ/mol	Joback Method
hf	-537.38	kJ/mol	Joback Method
hfus	32.52	kJ/mol	Joback Method
hvap	68.15	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.007		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	2379.00		NIST Webbook
rinpol	2379.00		NIST Webbook
tb	714.94	K	Joback Method
tc	919.70	K	Joback Method
tf	419.58	K	Joback Method
vc	0.853	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.91	J/mol×K	714.94	Joback Method
cpg	618.29	J/mol×K	749.07	Joback Method
cpg	632.75	J/mol×K	783.19	Joback Method
cpg	646.28	J/mol×K	817.32	Joback Method
cpg	658.90	J/mol×K	851.45	Joback Method
cpg	670.62	J/mol×K	885.57	Joback Method
cpg	681.44	J/mol×K	919.70	Joback Method
dvisc	0.0008995	Pa×s	419.58	Joback Method

dvisc	0.0004991	Pa×s	468.81	Joback Method
dvisc	0.0003098	Pa×s	518.03	Joback Method
dvisc	0.0002089	Pa×s	567.26	Joback Method
dvisc	0.0001500	Pa×s	616.49	Joback Method
dvisc	0.0001131	Pa×s	665.71	Joback Method
dvisc	0.0000887	Pa×s	714.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415078&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