3-(3-chloro, 4-isobutoxyphenyl)-2-methyl-propionic acid, methyl ester

Inchi: InChI=1S/C15H21ClO3/c1-10(2)9-19-14-6-5-12(8-13(14)16)7-11(3)15(17)18-4/h5-6,8,10
InchiKey: XXZOOMNHWNCCRK-UHFFFAOYSA-N
Formula: C15H21ClO3
SMILES: COC(=O)C(C)Cc1ccc(OCC(C)C)c(Cl)c1
Mol. weight [g/mol]: 284.78

Physical Properties

Property code	Value	Unit	Source
gf	-187.16	kJ/mol	Joback Method
hf	-542.66	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.726		Crippen Method
mcvol	224.000	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	1875.30		NIST Webbook
rinpol	1875.30		NIST Webbook
tb	714.50	K	Joback Method
tc	922.64	K	Joback Method
tf	404.58	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.43	J/mol×K	714.50	Joback Method
cpg	619.09	J/mol×K	749.19	Joback Method
cpg	633.78	J/mol×K	783.88	Joback Method
cpg	647.50	J/mol×K	818.57	Joback Method
cpg	660.28	J/mol×K	853.26	Joback Method
cpg	672.10	J/mol×K	887.95	Joback Method
cpg	683.00	J/mol×K	922.64	Joback Method
dvisc	0.0010634	Pa×s	404.58	Joback Method

dvisc	0.0005446	Pa×s	456.23	Joback Method
dvisc	0.0003196	Pa×s	507.89	Joback Method
dvisc	0.0002070	Pa×s	559.54	Joback Method
dvisc	0.0001442	Pa×s	611.19	Joback Method
dvisc	0.0001063	Pa×s	662.85	Joback Method
dvisc	0.0000819	Pa×s	714.50	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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