3-(3-Chloro-4-benzyloxy-phenyl)-2-methyl-propion acid, methyl ester

Inchi: InChI=1S/C18H19ClO3/c1-13(18(20)21-2)10-15-8-9-17(16(19)11-15)22-12-14-6-4-3-5-7-

InchiKey: XZSMKHFZBVXMAF-UHFFFAOYSA-N

Formula: C18H19ClO3

SMILES: COC(=O)C(C)Cc1ccc(OCc2ccccc2)c(Cl)c1

Mol. weight [g/mol]: 318.80

Physical Properties

Property code	Value	Unit	Source
gf	-47.05	kJ/mol	Joback Method
hf	-362.77	kJ/mol	Joback Method
hfus	34.33	kJ/mol	Joback Method
hvap	77.10	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.271		Crippen Method
mcvol	242.510	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	810.26	K	Joback Method
tc	1040.52	K	Joback Method
tf	479.81	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.83	J/mol×K	810.26	Joback Method
cpg	693.55	J/mol×K	848.64	Joback Method
cpg	707.02	J/mol×K	887.01	Joback Method
cpg	719.26	J/mol×K	925.39	Joback Method
cpg	730.30	J/mol×K	963.77	Joback Method
cpg	740.18	J/mol×K	1002.15	Joback Method
cpg	748.94	J/mol×K	1040.52	Joback Method
dvisc	0.0005947	Pa×s	479.81	Joback Method

dvisc	0.0003354	Pa×s	534.88	Joback Method
dvisc	0.0002105	Pa×s	589.96	Joback Method
dvisc	0.0001430	Pa×s	645.04	Joback Method
dvisc	0.0001033	Pa×s	700.11	Joback Method
dvisc	0.0000782	Pa×s	755.18	Joback Method
dvisc	0.0000615	Pa×s	810.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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