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

Inchi: InChI=1S/C17H17ClO3/c1-12(17(19)20-2)14-8-9-16(15(18)10-14)21-11-13-6-4-3-5-7-13/

InchiKey: BQLBOVHEXZBZFX-UHFFFAOYSA-N

Formula: C17H17ClO3

SMILES: COC(=O)C(C)c1ccc(OCc2ccccc2)c(Cl)c1

Mol. weight [g/mol]: 304.77

Physical Properties

Property code	Value	Unit	Source
gf	-55.47	kJ/mol	Joback Method
hf	-342.13	kJ/mol	Joback Method
hfus	31.74	kJ/mol	Joback Method
hvap	74.88	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.196		Crippen Method
mcvol	228.420	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	2240.10		NIST Webbook
tb	787.38	K	Joback Method
tc	1021.29	K	Joback Method
tf	468.54	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.46	J/mol×K	787.38	Joback Method
cpg	638.00	J/mol×K	826.36	Joback Method
cpg	651.30	J/mol×K	865.35	Joback Method
cpg	663.38	J/mol×K	904.33	Joback Method
cpg	674.28	J/mol×K	943.32	Joback Method
cpg	684.02	J/mol×K	982.30	Joback Method
cpg	692.64	J/mol×K	1021.29	Joback Method
dvisc	0.0006486	Pa×s	468.54	Joback Method
dvisc	0.0003706	Pa×s	521.68	Joback Method

dvisc	0.0002348	Pa×s	574.82	Joback Method
dvisc	0.0001607	Pa×s	627.96	Joback Method
dvisc	0.0001167	Pa×s	681.10	Joback Method
dvisc	0.0000888	Pa×s	734.24	Joback Method
dvisc	0.0000701	Pa×s	787.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157830&Units=SI

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