(3-Chloro-4-phenylpropoxy-phenyl)-acetic acid, methyl ester

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

InchiKey: KUQVOMJTSZJNMM-UHFFFAOYSA-N

Formula: C17H17ClO3

SMILES: COC(=O)Cc1ccc(OCCc2ccccc2)c(Cl)c1

Mol. weight [g/mol]: 304.77

Physical Properties

Property code	Value	Unit	Source
gf	-53.03	kJ/mol	Joback Method
hf	-336.85	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	75.26	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.677		Crippen Method
mcvol	228.420	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	2428.30		NIST Webbook
tb	787.82	K	Joback Method
tc	1017.80	K	Joback Method
tf	483.54	K	Joback Method
vc	0.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.88	J/mol×K	787.82	Joback Method
cpg	637.18	J/mol×K	826.15	Joback Method
cpg	650.29	J/mol×K	864.48	Joback Method
cpg	662.24	J/mol×K	902.81	Joback Method
cpg	673.06	J/mol×K	941.14	Joback Method
cpg	682.77	J/mol×K	979.47	Joback Method
cpg	691.41	J/mol×K	1017.80	Joback Method
dvisc	0.0005783	Pa×s	483.54	Joback Method
dvisc	0.0003515	Pa×s	534.25	Joback Method

dvisc	0.0002328	Pa×s	584.97	Joback Method
dvisc	0.0001647	Pa×s	635.68	Joback Method
dvisc	0.0001227	Pa×s	686.39	Joback Method
dvisc	0.0000951	Pa×s	737.11	Joback Method
dvisc	0.0000762	Pa×s	787.82	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=R158026&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