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

Inchi: InChI=1S/C17H23ClO3/c1-20-17(19)12-14-7-8-16(15(18)11-14)21-10-9-13-5-3-2-4-6-13/

InchiKey: JTCMYGCPMOWARO-UHFFFAOYSA-N

Formula: C17H23ClO3

SMILES: COC(=O)Cc1ccc(OCCC2CCCCC2)c(Cl)c1

Mol. weight [g/mol]: 310.82

Physical Properties

Property code	Value	Unit	Source
gf	-140.99	kJ/mol	Joback Method
hf	-519.06	kJ/mol	Joback Method
hfus	33.06	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.405		Crippen Method
mcvol	241.320	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2333.90		NIST Webbook
rinpol	2333.90		NIST Webbook
tb	780.69	K	Joback Method
tc	1004.95	K	Joback Method
tf	464.50	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.39	J/mol×K	780.69	Joback Method
cpg	724.96	J/mol×K	818.07	Joback Method
cpg	741.15	J/mol×K	855.44	Joback Method
cpg	755.98	J/mol×K	892.82	Joback Method
cpg	769.47	J/mol×K	930.20	Joback Method
cpg	781.63	J/mol×K	967.57	Joback Method
cpg	792.50	J/mol×K	1004.95	Joback Method
dvisc	0.0007724	Pa×s	464.50	Joback Method

dvisc	0.0004340	Pa×s	517.20	Joback Method
dvisc	0.0002713	Pa×s	569.90	Joback Method
dvisc	0.0001836	Pa×s	622.60	Joback Method
dvisc	0.0001321	Pa×s	675.29	Joback Method
dvisc	0.0000997	Pa×s	727.99	Joback Method
dvisc	0.0000781	Pa×s	780.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157969&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