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

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

InchiKey: AIELJRVNUROGAJ-UHFFFAOYSA-N

Formula: C17H23ClO3

SMILES: COC(=O)C(C)c1ccc(OCC2CCCCC2)c(Cl)c1

Mol. weight [g/mol]: 310.82

Physical Properties

Property code	Value	Unit	Source
gf	-143.43	kJ/mol	Joback Method
hf	-524.34	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	73.03	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.576		Crippen Method
mcvol	241.320	ml/mol	McGowan Method
pc	1820.06	kPa	Joback Method
rinpol	2232.20		NIST Webbook
rinpol	2232.20		NIST Webbook
tb	780.25	K	Joback Method
tc	1008.24	K	Joback Method
tf	449.50	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.93	J/mol×K	780.25	Joback Method
cpg	725.79	J/mol×K	818.25	Joback Method
cpg	742.21	J/mol×K	856.25	Joback Method
cpg	757.21	J/mol×K	894.24	Joback Method
cpg	770.82	J/mol×K	932.24	Joback Method
cpg	783.04	J/mol×K	970.24	Joback Method
cpg	793.91	J/mol×K	1008.24	Joback Method
dvisc	0.0008875	Pa×s	449.50	Joback Method

dvisc	0.0004643	Pa×s	504.62	Joback Method
dvisc	0.0002760	Pa×s	559.75	Joback Method
dvisc	0.0001801	Pa×s	614.88	Joback Method
dvisc	0.0001260	Pa×s	670.00	Joback Method
dvisc	0.0000931	Pa×s	725.12	Joback Method
dvisc	0.0000718	Pa×s	780.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R157845&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