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

Inchi: InChI=1S/C16H21ClO3/c1-19-16(18)10-13-7-8-15(14(17)9-13)20-11-12-5-3-2-4-6-12/h7-

InchiKey: KXICENYJWTTXKL-UHFFFAOYSA-N

Formula: C16H21ClO3

SMILES: COC(=O)Cc1ccc(OCC2CCCCC2)c(Cl)c1

Mol. weight [g/mol]: 296.79

Physical Properties

Property code	Value	Unit	Source
gf	-149.41	kJ/mol	Joback Method
hf	-498.42	kJ/mol	Joback Method
hfus	30.47	kJ/mol	Joback Method
hvap	71.19	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.015		Crippen Method
mcvol	227.230	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	2224.70		NIST Webbook
tb	757.81	K	Joback Method
tc	985.53	K	Joback Method
tf	453.23	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.92	J/mol×K	757.81	Joback Method
cpg	724.90	J/mol×K	947.58	Joback Method
cpg	712.76	J/mol×K	909.63	Joback Method
cpg	699.31	J/mol×K	871.67	Joback Method
cpg	684.53	J/mol×K	833.72	Joback Method
cpg	668.41	J/mol×K	795.76	Joback Method
cpg	735.74	J/mol×K	985.53	Joback Method
dvisc	0.0000890	Pa×s	757.81	Joback Method
dvisc	0.0001131	Pa×s	707.05	Joback Method

dvisc	0.0001492	Pa×s	656.28	Joback Method
dvisc	0.0002063	Pa×s	605.52	Joback Method
dvisc	0.0003025	Pa×s	554.76	Joback Method
dvisc	0.0004792	Pa×s	503.99	Joback Method
dvisc	0.0008415	Pa×s	453.23	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=R157974&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