3-Chloro-2-fluorobenzoic acid, cyclohexyl ester

Inchi: InChI=1S/C13H14ClFO2/c14-11-8-4-7-10(12(11)15)13(16)17-9-5-2-1-3-6-9/h4,7-9H,1-3,5

InchiKey: MDUVYNSQHOLDDV-UHFFFAOYSA-N

Formula: C13H14ClFO2

SMILES: O=C(OC1CCCCC1)c1cccc(Cl)c1F

Mol. weight [g/mol]: 256.70

Physical Properties

Property code	Value	Unit	Source
gf	-264.48	kJ/mol	Joback Method
hf	-500.39	kJ/mol	Joback Method
hfus	24.59	kJ/mol	Joback Method
hvap	61.28	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.969		Crippen Method
mcvol	180.860	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1853.00		NIST Webbook
tb	666.02	K	Joback Method
tc	899.53	K	Joback Method
tf	397.78	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.50	J/mol×K	666.02	Joback Method
cpg	485.97	J/mol×K	704.94	Joback Method
cpg	501.22	J/mol×K	743.86	Joback Method
cpg	515.28	J/mol×K	782.77	Joback Method
cpg	528.19	J/mol×K	821.69	Joback Method
cpg	539.97	J/mol×K	860.61	Joback Method
cpg	550.65	J/mol×K	899.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357723&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

Legend

cpg:	Ideal gas heat capacity
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