3-Chloro-2-fluorobenzoic acid, cyclohexylmethyl ester

Inchi: InChI=1S/C14H16ClFO2/c15-12-8-4-7-11(13(12)16)14(17)18-9-10-5-2-1-3-6-10/h4,7-8,1

InchiKey: CIXJCBZECJWMCV-UHFFFAOYSA-N

Formula: C14H16ClFO2

SMILES: O=C(OCC1CCCCC1)c1cccc(Cl)c1F

Mol. weight [g/mol]: 270.73

Physical Properties

Property code	Value	Unit	Source
gf	-256.06	kJ/mol	Joback Method
hf	-521.03	kJ/mol	Joback Method
hfus	27.18	kJ/mol	Joback Method
hvap	63.51	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.216		Crippen Method
mcvol	194.950	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	688.90	K	Joback Method
tc	917.92	K	Joback Method
tf	409.05	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.94	J/mol×K	688.90	Joback Method
cpg	538.77	J/mol×K	727.07	Joback Method
cpg	554.36	J/mol×K	765.24	Joback Method
cpg	568.74	J/mol×K	803.41	Joback Method
cpg	581.96	J/mol×K	841.58	Joback Method
cpg	594.03	J/mol×K	879.75	Joback Method
cpg	604.99	J/mol×K	917.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357726&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