3-Chloro-2-fluorobenzoic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C15H12ClFO2/c1-9-6-10(2)8-11(7-9)19-15(18)12-4-3-5-13(16)14(12)17/h3-8H

InchiKey: FMPLUYJMHVYCCO-UHFFFAOYSA-N

Formula: C15H12ClFO2

SMILES: Cc1cc(C)cc(OC(=O)c2cccc(Cl)c2F)c1

Mol. weight [g/mol]: 278.71

Physical Properties

Property code	Value	Unit	Source
gf	-178.94	kJ/mol	Joback Method
hf	-382.40	kJ/mol	Joback Method
hfus	31.20	kJ/mol	Joback Method
hvap	68.91	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.315		Crippen Method
mcvol	196.140	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2107.00		NIST Webbook
rinpol	2107.00		NIST Webbook
tb	728.87	K	Joback Method
tc	961.82	K	Joback Method
tf	464.40	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.22	J/mol×K	728.87	Joback Method
cpg	508.36	J/mol×K	767.69	Joback Method
cpg	520.50	J/mol×K	806.52	Joback Method
cpg	531.66	J/mol×K	845.34	Joback Method
cpg	541.85	J/mol×K	884.17	Joback Method
cpg	551.12	J/mol×K	922.99	Joback Method
cpg	559.48	J/mol×K	961.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357729&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/117-822-9/3-Chloro-2-fluorobenzoic-acid-3-5-dimethylphenyl-ester.pdf
Generated by Cheméo on 2024-04-30 08:22:11.507369866 +0000 UTC m=+16754580.427947177.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.