3-Chloro-2-fluorobenzamide, N-(2-iodo-4-methylphenyl)-

Inchi: InChI=1S/C14H10ClFINO/c1-8-5-6-12(11(17)7-8)18-14(19)9-3-2-4-10(15)13(9)16/h2-7H,

InchiKey: MRNYCFRHNSLKSQ-UHFFFAOYSA-N

Formula: C14H10ClFINO

SMILES: Cc1ccc(NC(=O)c2cccc(Cl)c2F)c(I)c1

Mol. weight [g/mol]: 389.59

Physical Properties

Property code	Value	Unit	Source
gf	65.15	kJ/mol	Joback Method
hf	-99.20	kJ/mol	Joback Method
hfus	36.92	kJ/mol	Joback Method
hvap	80.08	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.644		Crippen Method
mcvol	211.980	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	826.88	K	Joback Method
tc	1087.43	K	Joback Method
tf	541.62	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.47	J/mol×K	826.88	Joback Method
cpg	516.94	J/mol×K	870.30	Joback Method
cpg	526.45	J/mol×K	913.73	Joback Method
cpg	535.08	J/mol×K	957.15	Joback Method
cpg	542.91	J/mol×K	1000.58	Joback Method
cpg	550.01	J/mol×K	1044.00	Joback Method
cpg	556.47	J/mol×K	1087.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358140&Units=SI

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