3-Chloro-2-fluorobenzamide, N-(4-methoxyphenyl)-

Inchi: InChI=1S/C14H11ClFNO2/c1-19-10-7-5-9(6-8-10)17-14(18)11-3-2-4-12(15)13(11)16/h2-

InchiKey: VDLAKXHPYNDGGY-UHFFFAOYSA-N

Formula: C14H11ClFNO2

SMILES: COc1ccc(NC(=O)c2cccc(Cl)c2F)cc1

Mol. weight [g/mol]: 279.69

Physical Properties

Property code	Value	Unit	Source
gf	-88.34	kJ/mol	Joback Method
hf	-296.82	kJ/mol	Joback Method
hfus	34.09	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.740		Crippen Method
mcvol	192.030	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2438.00		NIST Webbook
rinpol	2438.00		NIST Webbook
tb	751.18	K	Joback Method
tc	985.49	K	Joback Method
tf	493.27	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.26	J/mol×K	751.18	Joback Method
cpg	506.43	J/mol×K	790.23	Joback Method
cpg	517.58	J/mol×K	829.28	Joback Method
cpg	527.74	J/mol×K	868.34	Joback Method
cpg	536.96	J/mol×K	907.39	Joback Method
cpg	545.25	J/mol×K	946.44	Joback Method
cpg	552.65	J/mol×K	985.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358136&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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