3-Chloro-2-fluorobenzamide, N-(2,5-dimethoxyphenyl)-

Inchi: InChI=1S/C15H13ClFNO3/c1-20-9-6-7-13(21-2)12(8-9)18-15(19)10-4-3-5-11(16)14(10)1

InchiKey: PJAHDKSWHYITCN-UHFFFAOYSA-N

Formula: C15H13ClFNO3

SMILES: COc1ccc(OC)c(NC(=O)c2cccc(Cl)c2F)c1

Mol. weight [g/mol]: 309.72

Physical Properties

Property code	Value	Unit	Source
gf	-194.55	kJ/mol	Joback Method
hf	-461.15	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	77.75	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.749		Crippen Method
mcvol	211.990	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	801.46	K	Joback Method
tc	1029.95	K	Joback Method
tf	539.29	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.96	J/mol×K	801.46	Joback Method
cpg	583.02	J/mol×K	839.54	Joback Method
cpg	594.02	J/mol×K	877.62	Joback Method
cpg	603.95	J/mol×K	915.70	Joback Method
cpg	612.84	J/mol×K	953.79	Joback Method
cpg	620.69	J/mol×K	991.87	Joback Method
cpg	627.50	J/mol×K	1029.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358138&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