Benzamide, 3-chloro-2-fluoro-N-(3-chloro-2-fluorobenzoyl)-N-m

Inchi: InChI=1S/C15H9Cl2F2NO2/c1-20(14(21)8-4-2-6-10(16)12(8)18)15(22)9-5-3-7-11(17)13(

InchiKey: RRZRNEUGDMUJDO-UHFFFAOYSA-N

Formula: C15H9Cl2F2NO2

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

Mol. weight [g/mol]: 344.14

Physical Properties

Property code	Value	Unit	Source
gf	-298.82	kJ/mol	Joback Method
hf	-507.08	kJ/mol	Joback Method
hfus	41.90	kJ/mol	Joback Method
hvap	78.86	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.184		Crippen Method
mcvol	215.830	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	809.46	K	Joback Method
tc	1040.60	K	Joback Method
tf	555.08	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.83	J/mol×K	809.46	Joback Method
cpg	559.01	J/mol×K	847.98	Joback Method
cpg	568.26	J/mol×K	886.51	Joback Method
cpg	576.65	J/mol×K	925.03	Joback Method
cpg	584.24	J/mol×K	963.55	Joback Method
cpg	591.08	J/mol×K	1002.08	Joback Method
cpg	597.23	J/mol×K	1040.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407835&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