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

Inchi: InChI=1S/C16H11Cl2F2NO2/c1-2-21(15(22)9-5-3-7-11(17)13(9)19)16(23)10-6-4-8-12(18

InchiKey: UTRAAGATPRKTMN-UHFFFAOYSA-N

Formula: C16H11Cl2F2NO2

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

Mol. weight [g/mol]: 358.17

Physical Properties

Property code	Value	Unit	Source
gf	-290.40	kJ/mol	Joback Method
hf	-527.72	kJ/mol	Joback Method
hfus	44.49	kJ/mol	Joback Method
hvap	81.08	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.574		Crippen Method
mcvol	229.920	ml/mol	McGowan Method
pc	2081.22	kPa	Joback Method
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
tb	832.34	K	Joback Method
tc	1060.33	K	Joback Method
tf	566.35	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.33	J/mol×K	832.34	Joback Method
cpg	612.90	J/mol×K	870.34	Joback Method
cpg	622.54	J/mol×K	908.34	Joback Method
cpg	631.31	J/mol×K	946.34	Joback Method
cpg	639.26	J/mol×K	984.34	Joback Method
cpg	646.47	J/mol×K	1022.33	Joback Method
cpg	652.98	J/mol×K	1060.33	Joback Method

Sources

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=U407836&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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