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

Inchi: InChI=1S/C22H23Cl2F2NO2/c1-3-5-8-14(4-2)13-27(21(28)15-9-6-11-17(23)19(15)25)22(

InchiKey: LVUSWUAWPPORAX-UHFFFAOYSA-N

Formula: C22H23Cl2F2NO2

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

Mol. weight [g/mol]: 442.33

Physical Properties

Property code	Value	Unit	Source
gf	-242.32	kJ/mol	Joback Method
hf	-656.84	kJ/mol	Joback Method
hfus	56.51	kJ/mol	Joback Method
hvap	94.05	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	6.771		Crippen Method
mcvol	314.460	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2740.00		NIST Webbook
rinpol	2740.00		NIST Webbook
tb	969.18	K	Joback Method
tc	1194.19	K	Joback Method
tf	618.97	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.17	J/mol×K	969.18	Joback Method
cpg	954.53	J/mol×K	1006.68	Joback Method
cpg	965.87	J/mol×K	1044.18	Joback Method
cpg	976.27	J/mol×K	1081.69	Joback Method
cpg	985.80	J/mol×K	1119.19	Joback Method
cpg	994.54	J/mol×K	1156.69	Joback Method
cpg	1002.58	J/mol×K	1194.19	Joback Method

Sources

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=U407842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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