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

Inchi: InChI=1S/C22H23Cl2F2NO2/c1-2-3-4-5-6-7-14-27(21(28)15-10-8-12-17(23)19(15)25)22(

InchiKey: IVWXKSXMKWKEGE-UHFFFAOYSA-N

Formula: C22H23Cl2F2NO2

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

Mol. weight [g/mol]: 442.33

Physical Properties

Property code	Value	Unit	Source
gf	-239.88	kJ/mol	Joback Method
hf	-651.56	kJ/mol	Joback Method
hfus	60.04	kJ/mol	Joback Method
hvap	94.44	kJ/mol	Joback Method
log10ws	-8.55		Crippen Method
logp	6.915		Crippen Method
mcvol	314.460	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	2862.00		NIST Webbook
rinpol	2862.00		NIST Webbook
tb	969.62	K	Joback Method
tc	1193.26	K	Joback Method
tf	633.97	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.72	J/mol×K	969.62	Joback Method
cpg	954.07	J/mol×K	1006.89	Joback Method
cpg	965.43	J/mol×K	1044.17	Joback Method
cpg	975.86	J/mol×K	1081.44	Joback Method
cpg	985.45	J/mol×K	1118.71	Joback Method
cpg	994.27	J/mol×K	1155.99	Joback Method
cpg	1002.41	J/mol×K	1193.26	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=U407844&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