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

Inchi: InChI=1S/C20H19Cl2F2NO2/c1-2-3-4-5-12-25(19(26)13-8-6-10-15(21)17(13)23)20(27)14

InchiKey: PRSJMWICWYGNGX-UHFFFAOYSA-N

Formula: C20H19Cl2F2NO2

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

Mol. weight [g/mol]: 414.27

Physical Properties

Property code	Value	Unit	Source
gf	-256.72	kJ/mol	Joback Method
hf	-610.28	kJ/mol	Joback Method
hfus	54.85	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.134		Crippen Method
mcvol	286.280	ml/mol	McGowan Method
pc	1506.98	kPa	Joback Method
rinpol	2646.00		NIST Webbook
rinpol	2646.00		NIST Webbook
tb	923.86	K	Joback Method
tc	1145.89	K	Joback Method
tf	611.43	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.46	J/mol×K	923.86	Joback Method
cpg	837.26	J/mol×K	960.86	Joback Method
cpg	848.09	J/mol×K	997.87	Joback Method
cpg	858.02	J/mol×K	1034.87	Joback Method
cpg	867.12	J/mol×K	1071.88	Joback Method
cpg	875.46	J/mol×K	1108.88	Joback Method
cpg	883.10	J/mol×K	1145.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407841&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