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

Inchi: InChI=1S/C21H21Cl2F2NO2/c1-2-3-4-5-6-13-26(20(27)14-9-7-11-16(22)18(14)24)21(28)

InchiKey: JLPHIFBTHJNEQZ-UHFFFAOYSA-N

Formula: C21H21Cl2F2NO2

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

Mol. weight [g/mol]: 428.30

Physical Properties

Property code	Value	Unit	Source
gf	-248.30	kJ/mol	Joback Method
hf	-630.92	kJ/mol	Joback Method
hfus	57.45	kJ/mol	Joback Method
hvap	92.21	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.525		Crippen Method
mcvol	300.370	ml/mol	McGowan Method
pc	1400.64	kPa	Joback Method
rinpol	2754.00		NIST Webbook
tb	946.74	K	Joback Method
tc	1169.15	K	Joback Method
tf	622.70	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.24	J/mol×K	946.74	Joback Method
cpg	895.32	J/mol×K	983.81	Joback Method
cpg	906.41	J/mol×K	1020.88	Joback Method
cpg	916.59	J/mol×K	1057.95	Joback Method
cpg	925.93	J/mol×K	1095.01	Joback Method
cpg	934.51	J/mol×K	1132.08	Joback Method
cpg	942.40	J/mol×K	1169.15	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=U407843&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