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

Inchi: InChI=1S/C23H25Cl2F2NO2/c1-2-3-4-5-6-7-8-15-28(22(29)16-11-9-13-18(24)20(16)26)2

InchiKey: VMVOMWOEAYGHNA-UHFFFAOYSA-N

Formula: C23H25Cl2F2NO2

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

Mol. weight [g/mol]: 456.35

Physical Properties

Property code	Value	Unit	Source
gf	-231.46	kJ/mol	Joback Method
hf	-672.20	kJ/mol	Joback Method
hfus	62.63	kJ/mol	Joback Method
hvap	96.66	kJ/mol	Joback Method
log10ws	-8.96		Crippen Method
logp	7.305		Crippen Method
mcvol	328.550	ml/mol	McGowan Method
pc	1219.14	kPa	Joback Method
rinpol	2969.00		NIST Webbook
rinpol	2969.00		NIST Webbook
tb	992.50	K	Joback Method
tc	1218.27	K	Joback Method
tf	645.24	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.85	J/mol×K	992.50	Joback Method
cpg	1013.50	J/mol×K	1030.13	Joback Method
cpg	1025.12	J/mol×K	1067.76	Joback Method
cpg	1035.81	J/mol×K	1105.38	Joback Method
cpg	1045.66	J/mol×K	1143.01	Joback Method
cpg	1054.73	J/mol×K	1180.64	Joback Method
cpg	1063.13	J/mol×K	1218.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407845&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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