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

Inchi: InChI=1S/C19H17Cl2F2NO2/c1-2-3-4-11-24(18(25)12-7-5-9-14(20)16(12)22)19(26)13-8-

InchiKey: YPVHKQIFOJBXQD-UHFFFAOYSA-N

Formula: C19H17Cl2F2NO2

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

Mol. weight [g/mol]: 400.25

Physical Properties

Property code	Value	Unit	Source
gf	-265.14	kJ/mol	Joback Method
hf	-589.64	kJ/mol	Joback Method
hfus	52.27	kJ/mol	Joback Method
hvap	87.76	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	5.744		Crippen Method
mcvol	272.190	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpol	2543.00		NIST Webbook
rinpol	2543.00		NIST Webbook
tb	900.98	K	Joback Method
tc	1123.42	K	Joback Method
tf	600.16	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.42	J/mol×K	900.98	Joback Method
cpg	779.95	J/mol×K	938.05	Joback Method
cpg	790.51	J/mol×K	975.13	Joback Method
cpg	800.18	J/mol×K	1012.20	Joback Method
cpg	809.03	J/mol×K	1049.28	Joback Method
cpg	817.12	J/mol×K	1086.35	Joback Method
cpg	824.51	J/mol×K	1123.42	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=U407840&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