

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

Inchi:	InChI=1S/C18H15Cl2F2NO2/c1-2-3-10-23(17(24)11-6-4-8-13(19)15(11)21)18(25)12-7-5
InchiKey:	OTTKMEALNZMXAX-UHFFFAOYSA-N
Formula:	C18H15Cl2F2NO2
SMILES:	CCCCN(C(=O)c1cccc(Cl)c1F)C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]:	386.22

Physical Properties

Property code	Value	Unit	Source
gf	-273.56	kJ/mol	Joback Method
hf	-569.00	kJ/mol	Joback Method
hfus	49.68	kJ/mol	Joback Method
hvap	85.53	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.354		Crippen Method
mcvol	258.100	ml/mol	McGowan Method
pc	1759.49	kPa	Joback Method
rinsol	2442.00		NIST Webbook
tb	878.10	K	Joback Method
tc	1101.70	K	Joback Method
tf	588.89	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.18	J/molxK	878.10	Joback Method
cpg	723.42	J/molxK	915.37	Joback Method
cpg	733.70	J/molxK	952.63	Joback Method
cpg	743.10	J/molxK	989.90	Joback Method
cpg	751.68	J/molxK	1027.17	Joback Method
cpg	759.50	J/molxK	1064.44	Joback Method
cpg	766.62	J/molxK	1101.70	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=U407838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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