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

Inchi: InChI=1S/C17H13Cl2F2NO2/c1-2-9-22(16(23)10-5-3-7-12(18)14(10)20)17(24)11-6-4-8-1

InchiKey: COQCPMUJPFWXIW-UHFFFAOYSA-N

Formula: C17H13Cl2F2NO2

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

Mol. weight [g/mol]: 372.19

Physical Properties

Property code	Value	Unit	Source
gf	-281.98	kJ/mol	Joback Method
hf	-548.36	kJ/mol	Joback Method
hfus	47.09	kJ/mol	Joback Method
hvap	83.31	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	4.964		Crippen Method
mcvol	244.010	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	855.22	K	Joback Method
tc	1080.69	K	Joback Method
tf	577.62	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.80	J/mol×K	855.22	Joback Method
cpg	667.72	J/mol×K	892.80	Joback Method
cpg	677.70	J/mol×K	930.38	Joback Method
cpg	686.80	J/mol×K	967.95	Joback Method
cpg	695.08	J/mol×K	1005.53	Joback Method
cpg	702.61	J/mol×K	1043.11	Joback Method
cpg	709.44	J/mol×K	1080.69	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407837&Units=SI

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