

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

Inchi: InChI=1S/C24H27Cl2F2NO2/c1-2-3-4-5-6-7-8-9-16-29(23(30)17-12-10-14-19(25)21(17)22-18)/N
InchiKey: VRSAEYKIDHRRJ-UHFFFAOYSA-N
Formula: C24H27Cl2F2NO2
SMILES: CCCCCCCCCN(C(=O)c1cccc(Cl)c1F)C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 470.38

Physical Properties

Property code	Value	Unit	Source
gf	-223.04	kJ/mol	Joback Method
hf	-692.84	kJ/mol	Joback Method
hfus	65.22	kJ/mol	Joback Method
hvap	98.89	kJ/mol	Joback Method
log10ws	-9.38		Crippen Method
logp	7.695		Crippen Method
mvol	342.640	ml/mol	McGowan Method
pc	1141.34	kPa	Joback Method
rinpol	3072.00		NIST Webbook
rinpol	3072.00		NIST Webbook
tb	1015.38	K	Joback Method
tc	1244.24	K	Joback Method
tf	656.51	K	Joback Method
vc	1.327	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1060.59	J/molxK	1015.38	Joback Method
cpg	1073.55	J/molxK	1053.52	Joback Method
cpg	1085.47	J/molxK	1091.67	Joback Method
cpg	1096.44	J/molxK	1129.81	Joback Method
cpg	1106.55	J/molxK	1167.95	Joback Method
cpg	1115.89	J/molxK	1206.09	Joback Method
cpg	1124.56	J/molxK	1244.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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