

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

Inchi: InChI=1S/C19H17Cl2F2NO2/c1-11(2)9-10-24(18(25)12-5-3-7-14(20)16(12)22)19(26)13-

InchiKey: WRZQDMLTQFRPLN-UHFFFAOYSA-N

Formula: C19H17Cl2F2NO2

SMILES: CC(C)CCN(C(=O)c1cccc(Cl)c1F)C(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 400.25

Physical Properties

Property code	Value	Unit	Source
gf	-267.58	kJ/mol	Joback Method
hf	-594.92	kJ/mol	Joback Method
hfus	48.74	kJ/mol	Joback Method
hvap	87.37	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	5.600		Crippen Method
mcvol	272.190	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	900.54	K	Joback Method
tc	1125.44	K	Joback Method
tf	585.16	K	Joback Method
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.97	J/mol×K	900.54	Joback Method
cpg	780.58	J/mol×K	938.02	Joback Method
cpg	791.20	J/mol×K	975.51	Joback Method
cpg	800.89	J/mol×K	1012.99	Joback Method
cpg	809.73	J/mol×K	1050.48	Joback Method
cpg	817.78	J/mol×K	1087.96	Joback Method
cpg	825.11	J/mol×K	1125.44	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U407839&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/112-690-1/Benzamide-3-chloro-2-fluoro-N-3-chloro-2-fluorobenzoyl-N-3-methylbutyl.pdf>

Generated by Cheméo on 2024-05-13 04:40:49.496363976 +0000 UTC m=+17864498.416941291.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.