

Benodanil

Other names:	2-Iodo-N-phenylbenzamide 2-Iodobenzanilide 2-Iodobenzoic acid anilide BAS 3170F BAS-3170 Benefit Benzamide, 2-iodo-N-phenyl- Benzanilide, 2-iodo- Calirus NSC 100499
Inchi:	InChI=1S/C13H10INO/c14-12-9-5-4-8-11(12)13(16)15-10-6-2-1-3-7-10/h1-9H,(H,15,16)
InchiKey:	LJOZMWRYMKECFF-UHFFFAOYSA-N
Formula:	C13H10INO
SMILES:	OC(=Nc1ccccc1)c1ccccc1I
Mol. weight [g/mol]:	323.13
CAS:	15310-01-7

Physical Properties

Property code	Value	Unit	Source
hf	147.01	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Joback Method
log10ws	-4.21		Estimated Solubility Method
logp	3.927		Crippen Method
mcvol	183.880	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
tb	817.06	K	Joback Method
tc	1081.55	K	Joback Method

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15310017&Units=SI

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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