

Pyridaben

Other names:	3(2H)-Pyridazinone,
Inchi:	4-chloro-2-(1,1-dimethylethyl)-5-[[[4-(1,1-dimethylethyl)phenyl]methyl]thio]-
InchiKey:	DWFZBUWUXWZWKD-UHFFFAOYSA-N
Formula:	C ₁₉ H ₂₅ ClN ₂ O ₂ S
SMILES:	CC(C)(C)c1ccc(CSc2cnn(C(C)(C)C)c(=O)c2Cl)cc1
Mol. weight [g/mol]:	364.93
CAS:	96489-71-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	5.241		Crippen Method
mcvol	285.470	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96489713&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/42-556-8/Pyridaben.pdf>

Generated by Cheméo on 2024-05-01 11:24:29.945574681 +0000 UTC m=+16851918.866151993.

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