

Rabenzazole

Other names:	1H-Benzimidazole, 2-(3,5-dimethyl-1H-pyrazol-1-yl)- 2-(3,5-Dimethylpyrazol-1-yl)-1H-benzimidazole 2-(3,5-dimethyl-1H-pyrazol-1-yl)-1H-benzimidazole
Inchi:	InChI=1S/C12H12N4/c1-8-7-9(2)16(15-8)12-13-10-5-3-4-6-11(10)14-12/h3-7H,1-2H3,(H,
InchiKey:	RUGYNGIMTAFTLP-UHFFFAOYSA-N
Formula:	C12H12N4
SMILES:	<chem>Cc1cc(C)n(-c2nc3ccccc3[nH]2)n1</chem>
Mol. weight [g/mol]:	212.25
CAS:	40341-04-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	1.884		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
rropol	2026.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40341046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rropol:	Non-polar retention indices

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