2-(3,5-Dimethylpyrazol-1-yl)-1H-benzimidazole

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: Cc1cc(C)n(-c2nc3ccccc3[nH]2)n1
Mol. weight [g/mol]: 212.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Cheméo Relay (1.0)
logp	1.884		Crippen Method
mcvol	161.480	ml/mol	McGowan Method
rinpol	2026.00		NIST Webbook
tf	509.86	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40341046&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

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

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point