5-Amino-1-phenylpyrazole-4-carbonitrile

Other names: 1H-Pyrazole-4-carbonitrile, 5-amino-1-phenyl-
5-Amino-1-phenylpyrazole-4-carbonitrile
5-amino-1-phenyl-1H-pyrazole-4-carbonitrile
Inchi: InChI=1S/C10H8N4/c11-6-8-7-13-14(10(8)12)9-4-2-1-3-5-9/h1-5,7H,12H2
InchiKey: MAKQREKUUHPPIS-UHFFFAOYSA-N
Formula: C10H8N4
SMILES: N#Cc1cnn(-c2ccccc2)c1N
Mol. weight [g/mol]: 184.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Cheméo Relay (1.0)
logp	1.326		Crippen Method
mcvol	139.860	ml/mol	McGowan Method
tf	445.04	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5334430&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):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point