

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

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