3,5-DIMETHYL-1-PHENYLPYRAZOLE

Other names: 3,5-Dimethyl-1-phenylpyrazole
3,5-dimethyl-1-phenyl-1H-pyrazole
Inchi: InChI=1S/C11H12N2/c1-9-8-10(2)13(12-9)11-6-4-3-5-7-11/h3-8H,1-2H3
InchiKey: ULPMPUPEFBDQQA-UHFFFAOYSA-N
Formula: C11H12N2
SMILES: Cc1cc(C)n(-c2ccccc2)n1
Mol. weight [g/mol]: 172.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.29		Cheméo Relay (1.0)
logp	2.489		Crippen Method
mcvol	142.590	ml/mol	McGowan Method
tb	560.81	K	Cheméo Relay (1.0)
tf	301.20	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.70	K	1.70	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1131164&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point