1H-Indole, 1,3-dimethyl-

Other names:	Indole, 1,3-dimethyl- 1,3-Dimethylindole
Inchi:	InChI=1S/C10H11N/c1-8-7-11(2)10-6-4-3-5-9(8)10/h3-7H,1-2H3
InchiKey:	NAPPMSNSLWACIV-UHFFFAOYSA-N
Formula:	C10H11N
SMILES:	Cc1cn(C)c2ccccc12
Mol. weight [g/mol]:	145.20
CAS:	875-30-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.04		Crippen Method
logp	2.487		Crippen Method
mcvol	122.820	ml/mol	McGowan Method
rinpol	1383.00		NIST Webbook
rinpol	1383.00		NIST Webbook
tb	531.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	0.90	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C875309&Units=SI
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure