Isoquinoline, 1-methyl-

Other names:	1-Methylisoquinoline
	Isoquinaldine
Inchi:	InChI=1S/C10H9N/c1-8-10-5-3-2-4-9(10)6-7-11-8/h2-7H,1H3
InchiKey:	PBYMYAJONQZORL-UHFFFAOYSA-N
Formula:	C10H9N
SMILES:	Cc1nccc2ccccc12
Mol. weight [g/mol]:	143.19
CAS:	1721-93-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	2.543		Crippen Method
mcvol	118.520	ml/mol	McGowan Method
rinpol	1326.00		NIST Webbook
rinpol	229.21		NIST Webbook
rinpol	1326.00		NIST Webbook
tb	521.20	K	NIST Webbook
tb	528.15 ± 0.70	K	NIST Webbook
tb	521.15 ± 2.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.20	K	2.10	NIST Webbook
tbrp	397.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39660e+01
Coeff. B	-4.06782e+03
Coeff. C	-8.60300e+01
Temperature range (K), min.	383.42
Temperature range (K), max.	556.05

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1721933&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure