

Quinoline, 3,6-dimethyl-

Other names:	3,6-dimethylquinoline
Inchi:	InChI=1S/C11H11N/c1-8-3-4-11-10(5-8)6-9(2)7-12-11/h3-7H,1-2H3
InchiKey:	XEDLZYLCKAHYHR-UHFFFAOYSA-N
Formula:	C11H11N
SMILES:	Cc1ccc2ncc(C)cc2c1
Mol. weight [g/mol]:	157.21
CAS:	20668-26-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.852		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
rinpol	1427.00		NIST Webbook
rinpol	1429.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1420.00		NIST Webbook
tf	331.00 ± 4.00	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.42407e+01
Coeff. B	-4.30975e+03
Coeff. C	-9.21460e+01
Temperature range (K), min.	401.02
Temperature range (K), max.	574.80

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=C20668262&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

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
tf:	Normal melting (fusion) point

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