Quinoline, 4,6-dimethyl-

Other names:	4,6-dimethylquinoline
Inchi:	InChI=1S/C11H11N/c1-8-3-4-11-10(7-8)9(2)5-6-12-11/h3-7H,1-2H3
InchiKey:	JTLZWQVUPZYROB-UHFFFAOYSA-N
Formula:	C11H11N
SMILES:	Cc1ccc2nccc(C)c2c1
Mol. weight [g/mol]:	157.21
CAS:	826-77-7

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	1472.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1472.00		NIST Webbook
ripol	2159.00		NIST Webbook
ripol	2133.00		NIST Webbook
ripol	2133.00		NIST Webbook
ripol	2159.00		NIST Webbook
tb	546.70	K	NIST Webbook
tb	548.00 ± 5.00	K	NIST Webbook
tb	546.00 ± 4.00	K	NIST Webbook
tb	548.00 ± 6.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39338e+01
Coeff. B	-4.22921e+03
Coeff. C	-9.27020e+01
Temperature range (K), min.	402.62
Temperature range (K), max.	583.20

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C826777&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

Latest version available from:

https://www.chemeo.com/cid/42-876-3/Quinoline-4-6-dimethyl.pdf

Generated by Cheméo on 2024-10-12 03:10:06.75741823 +0000 UTC m=+3283469.394387479.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.