Quinoline, 5,8-dimethyl-

Other names: 5,8-Dimethylquinoline
Inchi: InChI=1S/C11H11N/c1-8-5-6-9(2)11-10(8)4-3-7-12-11/h3-7H,1-2H3
InchiKey: VVLZEQKZPNOPNS-UHFFFAOYSA-N
Formula: C11H11N
SMILES: Cc1ccc(C)c2ncccc12
Mol. weight [g/mol]: 157.21
CAS: 2623-50-9

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	1422.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1427.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2038.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39606e+01
Coeff. B	-4.19469e+03
Coeff. C	-9.10340e+01
Temperature range (K), min.	397.82
Temperature range (K), max.	576.02

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=C2623509&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
ripol:	Polar retention indices