Quinoline, 5-methyl-

Other names: 5-Methylquinoline
Inchi: InChI=1S/C10H9N/c1-8-4-2-6-10-9(8)5-3-7-11-10/h2-7H,1H3
InchiKey: LMYVCXSKCQSIEQ-UHFFFAOYSA-N
Formula: C10H9N
SMILES: Cc1cccc2ncccc12
Mol. weight [g/mol]: 143.19
CAS: 7661-55-4

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	1355.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1355.00		NIST Webbook
ripol	2025.00		NIST Webbook
ripol	2025.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2054.00		NIST Webbook
ripol	2025.00		NIST Webbook
ripol	2054.00		NIST Webbook
tb	531.00 ± 2.00	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41490e+01
Coeff. B	-4.20908e+03
Coeff. C	-8.93660e+01
Temperature range (K), min.	393.02
Temperature range (K), max.	565.64

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7661554&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

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