Quinoline, 3-methyl-

Other names: 3-Methylquinoline
Inchi: InChI=1S/C10H9N/c1-8-6-9-4-2-3-5-10(9)11-7-8/h2-7H,1H3
InchiKey: DTBDAFLSBDGPEA-UHFFFAOYSA-N
Formula: C10H9N
SMILES: Cc1cnc2ccccc2c1
Mol. weight [g/mol]: 143.19
CAS: 612-58-8

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	1361.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1340.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	232.62		NIST Webbook
rinpol	232.47		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	232.62		NIST Webbook
ripol	2014.00		NIST Webbook
ripol	2014.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2014.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2042.00		NIST Webbook
tb	521.65 ± 3.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	55.80	kJ/mol	485.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53018e+01
Coeff. B	-4.83374e+03
Coeff. C	-6.91990e+01
Temperature range (K), min.	391.14
Temperature range (K), max.	553.04

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
KDB: https://www.cheric.org/files/research/kdb/mol/mol1366.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C612588&Units=SI

Legend

hvapt: Enthalpy of vaporization at a given temperature
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