Quinoline, 2-ethyl-

Other names: 2-Ethylquinoline
Inchi: InChI=1S/C11H11N/c1-2-10-8-7-9-5-3-4-6-11(9)12-10/h3-8H,2H2,1H3
InchiKey: XCIZVKSCLVSDHN-UHFFFAOYSA-N
Formula: C11H11N
SMILES: CCc1ccc2ccccc2n1
Mol. weight [g/mol]: 157.21
CAS: 1613-34-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.797		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
rinpol	1374.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1374.00		NIST Webbook
rinpol	1388.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1970.00		NIST Webbook
ripol	1993.00		NIST Webbook
ripol	1970.00		NIST Webbook
tb	518.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.70	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39589e+01
Coeff. B	-4.04786e+03
Coeff. C	-8.53350e+01
Temperature range (K), min.	381.42
Temperature range (K), max.	553.44

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=C1613349&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

tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure