Quinoline, 2-butyl-

Other names: 2-Butylquinoline
Inchi: InChI=1S/C13H15N/c1-2-3-7-12-10-9-11-6-4-5-8-13(11)14-12/h4-6,8-10H,2-3,7H2,1H3
InchiKey: GMZLALYCWQSOQS-UHFFFAOYSA-N
Formula: C13H15N
SMILES: CCCCc1ccc2ccccc2n1
Mol. weight [g/mol]: 185.26
CAS: 7661-39-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.68		Crippen Method
logp	3.577		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpol	1624.00		NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.27891e+01
Coeff. B	-3.93969e+03
Coeff. C	-9.54820e+01
Temperature range (K), min.	410.62
Temperature range (K), max.	622.35

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7661394&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