Quinoline, 6-ethyl-

Other names: 6-Ethylquinoline
Inchi: InChI=1S/C11H11N/c1-2-9-5-6-11-10(8-9)4-3-7-12-11/h3-8H,2H2,1H3
InchiKey: VDOYSQQOKJDYDR-UHFFFAOYSA-N
Formula: C11H11N
SMILES: CCc1ccc2ncccc2c1
Mol. weight [g/mol]: 157.21
CAS: 19655-60-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.797		Crippen Method
mcvol	132.610	ml/mol	McGowan Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37954e+01
Coeff. B	-4.12855e+03
Coeff. C	-9.01580e+01
Temperature range (K), min.	395.80
Temperature range (K), max.	576.79

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19655608&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure