

Quinoline, 8-ethyl-

Other names:	8-ethylquinoline
Inchi:	InChI=1S/C11H11N/c1-2-9-5-3-6-10-7-4-8-12-11(9)10/h3-8H,2H2,1H3
InchiKey:	WSNATRDCOFYLCB-UHFFFAOYSA-N
Formula:	C11H11N
SMILES:	CCc1cccc2cccnc12
Mol. weight [g/mol]:	157.21
CAS:	19655-56-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	2.797		Crippen Method
mccvol	132.610	ml/mol	McGowan Method
rinpol	1395.00		NIST Webbook
tb	529.00 ± 3.00	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.33126e+01
Coeff. B	-3.92789e+03
Coeff. C	-8.82540e+01
Temperature range (K), min.	389.82
Temperature range (K), max.	579.17

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C19655562&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb:	Normal Boiling Point Temperature

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