Quinoline, 4,8-dimethyl-

Inchi: InChI=1S/C11H11N/c1-8-6-7-12-11-9(2)4-3-5-10(8)11/h3-7H,1-2H3
InchiKey: DULGUAMZWACUFO-UHFFFAOYSA-N
Formula: C11H11N
SMILES: Cc1ccnc2c(C)cccc12
Mol. weight [g/mol]: 157.21
CAS: 13362-80-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.852		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
tb	531.70	K	NIST Webbook
tf	330.40 ± 0.70	K	NIST Webbook
tf	331.00 ± 4.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.70	K	1.60	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13362806&Units=SI
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point