Quinoline, 2,4-dimethyl-

Other names: 2,4-Dimethylquinoline
4-METHYLQUINALDINE
Inchi: InChI=1S/C11H11N/c1-8-7-9(2)12-11-6-4-3-5-10(8)11/h3-7H,1-2H3
InchiKey: ZTNANFDSJRRZRJ-UHFFFAOYSA-N
Formula: C11H11N
SMILES: Cc1cc(C)c2ccccc2n1
Mol. weight [g/mol]: 157.21
CAS: 1198-37-4

Physical Properties

Property code	Value	Unit	Source
af	0.3690		KDB
log10ws	-1.94		Aqueous Solubility Prediction Method
logp	2.852		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
pc	3900.00	kPa	KDB
rinpol	1446.00		NIST Webbook
rinpol	247.38		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	247.96		NIST Webbook
rinpol	247.38		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1454.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1434.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	2063.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2063.00		NIST Webbook

ripol	2088.00		NIST Webbook
ripol	2086.00		NIST Webbook
ripol	2088.00		NIST Webbook
tb	532.00 ± 7.00	K	NIST Webbook
tb	540.35 ± 0.06	K	NIST Webbook
tb	538.20	K	NIST Webbook
tb	540.40	K	KDB
tc	807.00	K	KDB
tf	330.00	K	KDB
tf	288.00 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	56.30	kJ/mol	500.50	NIST Webbook
rhol	1053.34	kg/m3	293.10	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41680e+01
Coeff. B	-4.26710e+03
Coeff. C	-9.13700e+01
Temperature range (K), min.	398.79
Temperature range (K), max.	573.17

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1371.mol
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1198374&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

af:	Acentric Factor
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point