Quinoline, 2,7-dimethyl-

Other names: 2,7-Dimethylquinoline
m-Toluquinaldine
Inchi: InChI=1S/C11H11N/c1-8-3-5-10-6-4-9(2)12-11(10)7-8/h3-7H,1-2H3
InchiKey: QXKPLNCZSFACPU-UHFFFAOYSA-N
Formula: C11H11N
SMILES: Cc1ccc2ccc(C)nc2c1
Mol. weight [g/mol]: 157.21
CAS: 93-37-8

Physical Properties

Property code	Value	Unit	Source
chs	-5935.00 ± 2.10	kJ/mol	NIST Webbook
hf	121.80 ± 3.00	kJ/mol	NIST Webbook
hfs	34.30 ± 2.60	kJ/mol	NIST Webbook
hsub	87.50 ± 1.50	kJ/mol	NIST Webbook
hsub	87.50	kJ/mol	NIST Webbook
hsub	87.50 ± 1.50	kJ/mol	NIST Webbook
log10ws	-1.94		Aqueous Solubility Prediction Method
log10ws	-1.94		Estimated Solubility Method
logp	2.852		Crippen Method
mcvol	132.610	ml/mol	McGowan Method
rinpol	1397.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1425.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	243.54		NIST Webbook
rinpol	244.04		NIST Webbook
rinpol	1402.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1392.00		NIST Webbook
ripol	2044.00		NIST Webbook

ripol	2036.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2018.00		NIST Webbook
ripol	2018.00		NIST Webbook
ripol	2044.00		NIST Webbook
ripol	2018.00		NIST Webbook
tb	537.70	K	NIST Webbook
tf	334.00 ± 3.00	K	NIST Webbook
tf	334.00 ± 2.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.70	K	0.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40117e+01
Coeff. B	-4.19963e+03
Coeff. C	-9.06170e+01
Temperature range (K), min.	396.62
Temperature range (K), max.	573.32

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93378&Units=SI

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

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point