Quinoline, 2,4,6-trimethyl-

Other names: 2,4,6-Trimethylquinoline
Inchi: InChI=1S/C12H13N/c1-8-4-5-12-11(6-8)9(2)7-10(3)13-12/h4-7H,1-3H3
InchiKey: ZXGXGZGKWSUMJK-UHFFFAOYSA-N
Formula: C12H13N
SMILES: Cc1ccc2nc(C)cc(C)c2c1
Mol. weight [g/mol]: 171.24
CAS: 2243-89-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	3.160		Crippen Method
mcvol	146.700	ml/mol	McGowan Method
rinpol	1539.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1525.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2180.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2180.00		NIST Webbook
ripol	2180.00		NIST Webbook
tb	554.70	K	NIST Webbook
tf	311.00 ± 3.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	420.20	K	1.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39556e+01
Coeff. B	-4.29305e+03
Coeff. C	-9.49260e+01
Temperature range (K), min.	409.02
Temperature range (K), max.	591.57

Sources

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=C2243892&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

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