Quinoline, 2,6,8-trimethyl-

Other names: 2,6,8-trimethylquinoline
Inchi: InChI=1S/C12H13N/c1-8-6-9(2)12-11(7-8)5-4-10(3)13-12/h4-7H,1-3H3
InchiKey: TYDCAWVQILIWGV-UHFFFAOYSA-N
Formula: C12H13N
SMILES: Cc1cc(C)c2nc(C)ccc2c1
Mol. weight [g/mol]: 171.24
CAS: 2243-90-5

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	1461.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1475.00		NIST Webbook
ripol	2040.00		NIST Webbook
ripol	2018.00		NIST Webbook
ripol	2018.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2018.00		NIST Webbook
ripol	2042.00		NIST Webbook
ripol	2018.00		NIST Webbook
ripol	2042.00		NIST Webbook
tb	533.00 ± 3.00	K	NIST Webbook
tf	319.00 ± 4.00	K	NIST Webbook

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=C2243905&Units=SI
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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