

Quinoline, 6-(1-methylpropyl)-

Other names:	sec-Butylquinoline Quinoline, 6-(sec-butyl)- mixed with 8-(sec-butyl)quinoline (4:1) 6- and 8-sec-Butylquinoline 6-Sec-butyl quinoline
Inchi:	InChI=1S/C13H15N/c1-3-10(2)11-6-7-13-12(9-11)5-4-8-14-13/h4-10H,3H2,1-2H3
InchiKey:	AUBLFWWZTFFBNU-UHFFFAOYSA-N
Formula:	C13H15N
SMILES:	CCC(C)c1ccc2ncccc2c1
Mol. weight [g/mol]:	185.26
CAS:	65442-31-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	3.748		Crippen Method
mcvol	160.790	ml/mol	McGowan Method
rinpol	1577.30		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1577.30		NIST Webbook
rinpol	1592.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2235.00		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=C65442311&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

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