Quinoline, 2-(tribromomethyl)-

Other names:	«alpha»,«alpha»,«alpha»-Tribromoquinaldine
	«omega» «omega» «omega»-Tribromoquinaldine
	2-(Tribromomethyl)quinoline
	2-(«alpha»,«alpha»,«alpha»-tribromomethyl)quinoline
Inchi:	InChI=1S/C10H6Br3N/c11-10(12,13)9-6-5-7-3-1-2-4-8(7)14-9/h1-6H
InchiKey:	UDYYQHILRSDDMP-UHFFFAOYSA-N
Formula:	C10H6Br3N
SMILES:	BrC(Br)(Br)c1ccc2ccccc2n1
Mol. weight [g/mol]:	379.87
CAS:	613-53-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	4.530		Crippen Method
mcvol	171.020	ml/mol	McGowan Method

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=C613536&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

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