Quinoline, 8-bromo-

Inchi: InChI=1S/C9H6BrN/c10-8-5-1-3-7-4-2-6-11-9(7)8/h1-6H
InchiKey: PIWNKSHCLTZKSZ-UHFFFAOYSA-N
Formula: C9H6BrN
SMILES: Brc1cccc2cccnc12
Mol. weight [g/mol]: 208.06
CAS: 16567-18-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	2.997		Crippen Method
mcvol	121.930	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.70	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16567183&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tbrp: Boiling point at reduced pressure