

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
mcpvol	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/ci9903071>
Crippen Method: https://www.chemed.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

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