3-Benzylquinoline

Inchi: InChI=1S/C16H13N/c1-2-6-13(7-3-1)10-14-11-15-8-4-5-9-16(15)17-12-14/h1-9,11-12H,1
InchiKey: QVMSGEZMPYTLKN-UHFFFAOYSA-N
Formula: C16H13N
SMILES: c1ccc(Cc2cnc3ccccc3c2)cc1
Mol. weight [g/mol]: 219.28
CAS: 37045-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.14		Crippen Method
logp	3.826		Crippen Method
mcvol	179.300	ml/mol	McGowan Method
tf	339.00 ± 1.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	499.00	K	2.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37045162&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tf:	Normal melting (fusion) point