6-Benzylquinoline

Other names: Quinoline, 6-(phenylmethyl)-
Inchi: InChI=1S/C16H13N/c1-2-5-13(6-3-1)11-14-8-9-16-15(12-14)7-4-10-17-16/h1-10,12H,11H
InchiKey: GMGJJCVVIGBOAJ-UHFFFAOYSA-N
Formula: C16H13N
SMILES: c1ccc(Cc2ccc3ncccc3c2)cc1
Mol. weight [g/mol]: 219.28
CAS: 54884-99-0

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	352.50 ± 0.50	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.70	K	0.10	NIST Webbook
tbrp	413.50 ± 1.50	K	0.10	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=C54884990&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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point