Isoquinoline, 1-(phenylmethyl)-

Other names:	Isoquinoline, 1-benzyl-
	1-Benzylisoquinoline
Inchi:	InChI=1S/C16H13N/c1-2-6-13(7-3-1)12-16-15-9-5-4-8-14(15)10-11-17-16/h1-11H,12H2
InchiKey:	IZTUINVRJSCOIR-UHFFFAOYSA-N
Formula:	C16H13N
SMILES:	c1ccc(Cc2nccc3ccccc23)cc1
Mol. weight [g/mol]:	219.28
CAS:	6907-59-1

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	329.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	485.20	K	1.50	NIST Webbook
tbrp	485.00 ± 1.00	K	1.50	NIST Webbook
tbrp	418.00 ± 5.00	K	0.10	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6907591&Units=SI

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