

Pyridine, 3-(phenylmethyl)-

Other names:	3-Benzylpyridine Pyridine, 3-benzyl-
Inchi:	InChI=1S/C12H11N/c1-2-5-11(6-3-1)9-12-7-4-8-13-10-12/h1-8,10H,9H2
InchiKey:	UUCLVSDUMKMSM-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	c1ccc(Cc2cccnc2)cc1
Mol. weight [g/mol]:	169.22
CAS:	620-95-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.672		Crippen Method
mcvol	142.400	ml/mol	McGowan Method
rinpol	1497.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	560.70	K	NIST Webbook
tf	307.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	559.20	K	98.70	NIST Webbook
tbrp	559.00	K	98.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C620951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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