Pyridine, 2-(phenylmethyl)-

Other names:	2-Benzylpyridine
	Pyridine, 2-benzyl-
Inchi:	InChI=1S/C12H11N/c1-2-6-11(7-3-1)10-12-8-4-5-9-13-12/h1-9H,10H2
InchiKey:	PCFUWBOSXMKGIP-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	c1ccc(Cc2ccccn2)cc1
Mol. weight [g/mol]:	169.22
CAS:	101-82-6

Physical Properties

Property code	Value	Unit	Source
hvap	69.90 ± 2.80	kJ/mol	NIST Webbook
log10ws	-3.34		Crippen Method
logp	2.672		Crippen Method
mcvol	142.400	ml/mol	McGowan Method
rinpol	1439.20		NIST Webbook
rinpol	1432.00		NIST Webbook
rinpol	1482.00		NIST Webbook
ripol	2168.00		NIST Webbook
tb	549.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	69.80	kJ/mol	298.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	549.20	K	98.90	NIST Webbook
tbrp	549.00	K	98.90	NIST Webbook
tbrp	366.50 ± 0.50	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Heterocycles and Related Compounds:	https://www.doi.org/10.1021/je900034d
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure