

Pyridine, 4-(phenylmethyl)-

Other names:	Pyridine, 4-(phenylmethyl)- «gamma»-Benzylpyridine Ba 33216 4-Benzylpyridine
Inchi:	InChI=1S/C12H11N/c1-2-4-11(5-3-1)10-12-6-8-13-9-7-12/h1-9H,10H2
InchiKey:	DBOLXXRVIFGDTI-UHFFFAOYSA-N
Formula:	C12H11N
SMILES:	c1ccc(Cc2ccncc2)cc1
Mol. weight [g/mol]:	169.23

Physical Properties

Property code	Value	Unit	Source
af	0.4260		Cheméo Relay (1.0)
hf	244.98	kJ/mol	Cheméo Relay (1.0)
hvap	72.63	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	-1.80		Cheméo Relay (1.0)
logp	2.672		Crippen Method
mcvol	142.400	ml/mol	McGowan Method
pc	3630.19	kPa	Cheméo Relay (1.0, beta)
tb	564.77	K	Cheméo Relay (1.0)
tc	805.60	K	Cheméo Relay (1.0)
tf	290.09	K	Cheméo Relay (1.0)
vc	0.534	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2116656&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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