

2-Ethynyl pyridine

Inchi: InChI=1S/C7H5N/c1-2-7-5-3-4-6-8-7/h1,3-6H
InchiKey: NHUBNHMFXQNNMV-UHFFFAOYSA-N
Formula: C7H5N
SMILES: C#Cc1ccccn1
Mol. weight [g/mol]: 103.12
CAS: 1945-84-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	1.063		Crippen Method
mcpvol	87.110	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.50 ± 0.50	K	1.90	NIST Webbook
tbrp	358.00	K	4.30	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1945842&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcpvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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