

2-Pyridineethanamine

Other names:	2-(2-Aminoethyl)pyridine «alpha»-Pyridylethylamine Demethylbetahistine Pyridine, 2-(2-aminoethyl)- 2-(«beta»-Aminoethyl)pyridine 2-(2-Pyridyl)ethylamine 2-(2'-Aminoethyl)pyridine 2-Pyridylethylamine 2-(2-Pyridinyl)ethanamine 2-Aminoethylpyridine NSC 71989 Lilly 04432
Inchi:	InChI=1S/C7H10N2/c8-5-4-7-3-1-2-6-9-7/h1-3,6H,4-5,8H2
InchiKey:	XPQIPUZPSLAZDV-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	NCCc1ccccn1
Mol. weight [g/mol]:	122.17
CAS:	2706-56-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	0.583		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	1147.00		NIST Webbook
ripol	1768.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	365.70	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2706561&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure

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