

Tryptamine

Other names:	1H-Indole-3-ethanamine Indole, 3-(2-aminoethyl)- «beta»-(3-Indolyl)ethylamine Indol-3-ethylamine Tryptamin 2-(3-Indolyl)ethylamine 3-(2-Aminoethyl)indole (Amino-2 ethyl)-3 indole 3-Indoleethylamine 2-(indol-3-yl)ethylamine
Inchi:	InChI=1S/C10H12N2/c11-6-5-8-7-12-10-4-2-1-3-9(8)10/h1-4,7,12H,5-6,11H2
InchiKey:	APJYDQYYACXCRM-UHFFFAOYSA-N
Formula:	C10H12N2
SMILES:	NCCc1c[nH]c2ccccc12
Mol. weight [g/mol]:	160.22
CAS:	61-54-1

Physical Properties

Property code	Value	Unit	Source
ie	7.69 ± 0.08	eV	NIST Webbook
log10ws	-2.73		Crippen Method
logp	1.187		Crippen Method
mcvol	132.800	ml/mol	McGowan Method
rinpol	1750.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1775.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.20	K	0.03	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61541&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure

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