

Prolintane

Other names:

Pyrrolidine, 1-[1-(phenylmethyl)butyl]-
Pyrrolidine, 1-(«alpha»-propylphenethyl)-
1-Phenyl-2-pyrrolidinylpentane
Prolintan
1-(«alpha»-Propylphenethyl)pyrrolidine
1-[1-(Phenylmethyl)butyl] pyrrolidine
Phenylpyrrolidinopentane
Pyrrolidine, 1-(1-benzylbutyl)-

Inchi:

InChI=1S/C15H23N/c1-2-8-15(16-11-6-7-12-16)13-14-9-4-3-5-10-14/h3-5,9-10,15H,2,6-8

InchiKey:

OJCPSBCUMRIPFL-UHFFFAOYSA-N

Formula:

C15H23N

SMILES:

CCCC(Cc1cccc1)N1CCCC1

Mol. weight [g/mol]:

217.35

CAS:

493-92-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	3.494		Crippen Method
mcvol	197.570	ml/mol	McGowan Method
rinpol	1623.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1639.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1605.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1649.00		NIST Webbook
ripol	2000.00		NIST Webbook
ripol	2011.00		NIST Webbook
ripol	2017.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C493925&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
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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