

Procyclidine

Other names:

1-Pyrrolidinepropanol, «alpha»-cyclohexyl-«alpha»-phenyl-
Elorine
Kemadrin
Kemadrine
Lergine
Tricoloid
Tricyclamol
Vagosin
Arpicolin
Metanin
Osnervan
Procidlidina
Procyklidin
Prosyklidin
Spamol
Triciclidina
Triciloid
1-Cyclohexyl-1-phenyl-3-(1-pyrrolidiny)-1-propanol
1-Cyclohexyl-1-phenyl-3-pyrrolidino-1-propanol
«alpha»-Cyclohexyl-«alpha»-phenyl-1-pyrrolidinepropanol
NSC 169103

Inchi:

InChI=1S/C19H29NO/c21-19(17-9-3-1-4-10-17,18-11-5-2-6-12-18)13-16-20-14-7-8-15-20

InchiKey:

WYDUSKDSKCASEF-UHFFFAOYSA-N

Formula:

C19H29NO

SMILES:

OC(CCN1CCCC1)(c1ccccc1)C1CCCCC1

Mol. weight [g/mol]:

287.44

CAS:

77-37-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	3.940		Crippen Method
mcvol	248.940	ml/mol	McGowan Method
rinpol	2205.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2135.00		NIST Webbook

rinpol	2154.00	NIST Webbook
rinpol	2156.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2160.00	NIST Webbook
rinpol	2154.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2160.00	NIST Webbook

Sources

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=C77372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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