PROCYCLIDINE

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

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]: 287.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Cheméo Relay (1.0)
logp	3.940		Crippen Method
mcvol	248.940	ml/mol	McGowan Method
rinpol	2154.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2154.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2175.00		NIST Webbook

rinpol	2135.00		NIST Webbook
rinpol	2205.00		NIST Webbook
rinpol	2156.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2177.00		NIST Webbook
tb	649.78	K	Cheméo Relay (1.0)
tf	384.93	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77372&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point