

Phendimetrazine

Other names:	Bontril (+)-Phendimetrazine Morpholine, 3,4-dimethyl-2-phenyl-, (2S-trans)- Morpholine, 3,4-dimethyl-2-phenyl-, (+)- (+)-3,4-Dimethyl-2-phenylmorpholine D-2-phenyl-3,4-dimethylmorpholine Antapentan Mephenmetrazine Sedafamen Adphen (base) Bacarate (2S,3S)-3,4-Dimethyl-2-phenylmorpholine NSC 169187 (2S-trans)-3,4-Dimethyl-2-phenylmorpholine Phendimetrazine
Inchi:	InChI=1S/C12H17NO/c1-10-12(14-9-8-13(10)2)11-6-4-3-5-7-11/h3-7,10,12H,8-9H2,1-2H
InchiKey:	MFOCDFTXLCYLKU-UHFFFAOYSA-N
Formula:	C12H17NO
SMILES:	CC1C(c2ccccc2)OCCN1C
Mol. weight [g/mol]:	191.27
CAS:	634-03-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	2.078		Crippen Method
mcvol	161.170	ml/mol	McGowan Method
rinpol	1485.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1434.00		NIST Webbook

rinpol	1485.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1450.00	NIST Webbook
rinpol	1444.00	NIST Webbook
rinpol	1500.00	NIST Webbook
rinpol	1445.00	NIST Webbook
rinpol	1450.00	NIST Webbook
ripol	2002.00	NIST Webbook
ripol	2017.00	NIST Webbook
ripol	2047.00	NIST Webbook
ripol	2057.00	NIST Webbook
ripol	1963.00	NIST Webbook
ripol	1963.00	NIST Webbook
ripol	2009.00	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=C634037&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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