1-Piperidinecarbothioic acid, S-(1-methyl-1-phenylethyl) ester

Other names: Dimepiperate
S-(1-methyl-1-phenylethyl) piperidine-1-carbothioate
Inchi: InChI=1S/C15H21NOS/c1-15(2,13-9-5-3-6-10-13)18-14(17)16-11-7-4-8-12-16/h3,5-6,9-1
InchiKey: BWUPSGJXXPATLU-UHFFFAOYSA-N
Formula: C15H21NOS
SMILES: CC(C)(SC(=O)N1CCCCC1)c1ccccc1
Mol. weight [g/mol]: 263.40
CAS: 61432-55-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Crippen Method
logp	4.261		Crippen Method
mcvol	215.490	ml/mol	McGowan Method
rinpol	2082.00		NIST Webbook
rinpol	2088.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2093.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2082.00		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=C61432551&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