

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 |
| mvol | 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/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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