Meperidine

Other names:

1-Methyl-4-phenyl-4-piperidinecarboxylic acid ethyl ester
1-Methyl-4-phenyl-piperidin-4-carbon-saeure-aethylester
1-Methyl-4-phenylisonipecotic acid, ethyl ester
1-Methyl-4-phenylpiperidine-4-carboxylic acid ethyl ester
1-Methyl-4-phenylpiperidine-4-carboxylic acid ethyl ester (meperidine)
4-Piperidinecarboxylic acid, 1-methyl-4-phenyl-, ethyl ester
Centralgin
Demarol
Demerol
Dispadol
Dolantin
Dolcontral
Dolosal
Dolsin
Ethyl 1-methyl-4-phenyl-4-piperidinecarboxylate
Ethyl 1-methyl-4-phenylisonipecotate
Ethyl 1-methyl-4-phenylpiperidine-4-carboxylate
Isonipecaine
Isonipecotic acid, 1-methyl-4-phenyl-, ethyl ester
Lidol
Lydol
Meperidine (demerol))
Meperidol
Methyl phenylpiperidine carbonic acid ethyl ester
N-Methyl-4-phenyl-4-carbethoxypiperidine
Nemerol
Operidine
Petantin
Pethanol
Pethidin
Pethidine
Pethidine-M
Pethidineter
Petydyna
Phetidine
Piperosal
Pipersal
Piridosal
Renaudin

Inchi:

InChI=1S/C15H21NO2/c1-3-18-14(17)15(9-11-16(2)12-10-15)13-7-5-4-6-8-13/h4-8H,3,9-

InchiKey: XADCESSVHJOZHK-UHFFFAOYSA-N
Formula: C15H21NO2
SMILES: CCOC(=O)C1(c2ccccc2)CCN(C)CC1
Mol. weight [g/mol]: 247.33
CAS: 57-42-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Aqueous Solubility Prediction Method
logp	2.213		Crippen Method
mcvol	205.010	ml/mol	McGowan Method
rinpol	1755.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1741.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1789.40		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1751.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1730.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1767.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1734.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1740.00		NIST Webbook

rinpol	1720.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1751.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1751.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1739.00		NIST Webbook
rinpol	1731.00		NIST Webbook
rinpol	1789.40		NIST Webbook
ripol	2332.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2310.00		NIST Webbook
ripol	2332.00		NIST Webbook
tf	501.90	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.60	kJ/mol	308.20	NIST Webbook

Sources

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57421&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
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
tf:	Normal melting (fusion) point