

Etoperidone

Other names:

Inchi:	2-[3-[4-(3-chlorophenyl)piperazin-1-yl]propyl]-4,5-diethyl-2,4-dihydro-3H-1,2,4-triazol-3-one monohydrochloride
InchiKey:	IZBNCFOBMGTQX-UHFFFAOYSA-N
Formula:	C ₁₉ H ₂₈ ClN ₅ O
SMILES:	CCc1nn(CCCN2CCN(c3cccc(Cl)c3)CC2)c(=O)n1CC
Mol. weight [g/mol]:	377.91
CAS:	57775-22-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	2.493		Crippen Method
mcvol	292.500	ml/mol	McGowan Method
rinpol	3103.00		NIST Webbook
rinpol	3103.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57775221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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