

Indol-4(5H)-one, 3-ethyl-6,7-dihydro-2-methyl-5-(morpholinomethyl)

Other names:	EN-1733A Molindone 3-Ethyl-6,7-dihydro-2-methyl-5-(morpholinomethyl)indol-4(5H)-one
Inchi:	InChI=1S/C16H24N2O2/c1-3-13-11(2)17-14-5-4-12(16(19)15(13)14)10-18-6-8-20-9-7-18
InchiKey:	KLPWJLBORRMFGK-UHFFFAOYSA-N
Formula:	C16H24N2O2
SMILES:	CCc1c(C)[nH]c2c1C(=O)C(CN1CCOCC1)CC2
Mol. weight [g/mol]:	276.37
CAS:	7416-34-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.481		Crippen Method
mcvol	222.520	ml/mol	McGowan Method
rinpol	2465.00		NIST Webbook
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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=C7416344&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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