

Flunitrazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 5-(2-fluorophenyl)-1,3-dihydro-1-methyl-7-nitro- 2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-5-(2-fluorophenyl)-1-methyl-7-nitro- 1,3-Dihydro-5-(o-fluorophenyl)-1-methyl-7-nitro-2H-1,4-benzodiazepin-2-one 1-Methyl-7-nitro-5-(2-fluorophenyl)-3H-1,4-benzodiazepin-2(1H)-one Narcozep Ro 5-4200 Rohypnol 5-(o-Fluorophenyl)-1,3-dihydro-1-methyl-7-nitro-2H-1,4-benzodiazepin-2-one Roipnol 5-(2-Fluorophenyl)-1-methyl-7-nitro-1,3-dihydrobenzo[e][1,4]diazepin-2-one
Inchi:	InChI=1S/C16H12FN3O3/c1-19-14-7-6-10(20(22)23)8-12(14)16(18-9-15(19)21)11-4-2-3
InchiKey:	PPTYJKAXVCCBDU-UHFFFAOYSA-N
Formula:	C16H12FN3O3
SMILES:	CN1C(=O)CN=C(c2ccccc2F)c2cc([N+](=O)[O-])ccc21
Mol. weight [g/mol]:	313.28
CAS:	1622-62-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	2.548		Crippen Method
mcvol	214.340	ml/mol	McGowan Method
rinpol	2572.00		NIST Webbook
rinpol	2633.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2571.00		NIST Webbook
rinpol	2610.00		NIST Webbook
rinpol	2646.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2712.70		NIST Webbook
rinpol	2594.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2572.00		NIST Webbook
rinpol	2645.00		NIST Webbook
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
rinpol	2607.00		NIST Webbook

rinpol	2577.00	NIST Webbook
rinpol	2645.00	NIST Webbook
rinpol	2712.70	NIST Webbook
rinpol	2600.00	NIST Webbook
rinpol	2646.00	NIST Webbook
rinpol	2645.00	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=C1622624&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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