

2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-(2-fluorophenyl)-1-(2-hydroxyethyl)-

Other names:

Ro 7-2750

7-Chloro-5-(2-fluorophenyl)-1-(2-hydroxyethyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one

2-Hydroxyethylflurazepam

Flurazepam, hydroxyethyl

Flurazepam, (N-hydroxyethyl)-

N-1-(Hydroxyethyl)flurazepam

Flurazepam M (N-hydroxyethyl)

Inchi: InChI=1S/C17H14ClFN2O2/c18-11-5-6-15-13(9-11)17(12-3-1-2-4-14(12)19)20-10-16(23)

InchiKey: FOGBRQQHNOKOJQ-UHFFFAOYSA-N

Formula: C17H14ClFN2O2

SMILES: O=C1CN=C(c2ccccc2F)c2cc(Cl)ccc2N1CCO

Mol. weight [g/mol]: 332.76

CAS: 20971-53-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	2.655		Crippen Method
mcvol	229.120	ml/mol	McGowan Method
rinpol	2715.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2766.70		NIST Webbook
rinpol	2688.00		NIST Webbook
rinpol	2715.00		NIST Webbook
rinpol	2730.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C20971533&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpolar:	Non-polar retention indices

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