

HYDROXYETHYLFLURAZEPAM

Other names:	3-Hydroxyethylflurazepam
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:	JRCYGROYIMMPPO-UHFFFAOYSA-N
Formula:	C17H14ClFN2O2
SMILES:	O=C1CN=C(c2ccccc2F)c2cc(Cl)ccc2N1CCO
Mol. weight [g/mol]:	332.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Cheméo Relay (1.0)
logp	2.655		Crippen Method
mcvol	229.120	ml/mol	McGowan Method
tf	416.24	K	Cheméo Relay (1.0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20971533&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/123-037-4/HYDROXYETHYLFLURAZEPAM.pdf>

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