

Triazolam

Other names:

4H-[1,2,4]Triazolo[4,3-a][1,4]benzodiazepine,
8-chloro-6-(2-chlorophenyl)-1-methyl-
4H-s-Triazolo(4,3-a)(1,4)benzodiazepine, 8-chloro-6-(o-chlorophenyl)-1-methyl-

8-Chloro-6-(2-chlorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine
(triazolam)
8-Chloro-6-(2-chlorophenyl)-1-methyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine

8-Chloro-6-(o-chlorophenyl)-1-methyl-4H-s-triazolo(4,3-a)(1,4)benzodiazepine

Halcion

Novodorm

Songar

U 33030

U-33,030

Inchi: InChI=1S/C17H12Cl2N4/c1-10-21-22-16-9-20-17(12-4-2-3-5-14(12)19)13-8-11(18)6-7-15

InchiKey: JOFWLTCLBGQGBO-UHFFFAOYSA-N

Formula: C17H12Cl2N4

SMILES: Cc1nnc2n1-c1ccc(Cl)cc1C(c1ccccc1Cl)=NC2

Mol. weight [g/mol]: 343.21

CAS: 28911-01-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Aqueous Solubility Prediction Method
log10ws	-4.09		Estimated Solubility Method
logp	4.234		Crippen Method
mcvol	232.650	ml/mol	McGowan Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
rinpol	2992.00		NIST Webbook
rinpol	3007.00		NIST Webbook
rinpol	3187.00		NIST Webbook
rinpol	3017.00		NIST Webbook
rinpol	3008.00		NIST Webbook
rinpol	3008.00		NIST Webbook
rinpol	3017.00		NIST Webbook
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
rinpol	3017.00		NIST Webbook

rinpol	3020.00		NIST Webbook
rinpol	3023.00		NIST Webbook
rinpol	3000.00		NIST Webbook
rinpol	3010.00		NIST Webbook
rinpol	3018.00		NIST Webbook
rinpol	3020.00		NIST Webbook
rinpol	3043.00		NIST Webbook
tf	504.65	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	41.00	kJ/mol	514.50	NIST Webbook

Sources

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

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C28911015&Units=SI>

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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