

Prazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 7-chloro-1-(cyclopropylmethyl)-1,3-dihydro-5-phenyl-Demetrin W 4020 K-373 Lysanxia Trepidant Verstran 2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-1-(cyclopropylmethyl)-5-phenyl-7-Chloro-1-(cyclopropylmethyl)-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one 7-Chloro-1-cyclopropylmethyl-5-phenyl-1H-1,4-benzodiazepin-2(3H)-one Centrax Prazeeene Prazene Sedapran Settima NSC 277179 1-(Cyclopropylmethyl)-5-phenyl-7-chloro-1,3-dihydro-2H-1,4-benzodiazepin-2-one (prazepam)
Inchi:	INCHEM=C19H17CIN2O/c20-15-8-9-17-16(10-15)19(14-4-2-1-3-5-14)21-11-18(23)22(17)
InchiKey:	MWQCHHACWWAQLJ-UHFFFAOYSA-N
Formula:	C19H17CIN2O
SMILES:	O=C1CN=C(c2ccccc2)c2cc(Cl)ccc2N1CC1CC1
Mol. weight [g/mol]:	324.80
CAS:	2955-38-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.43		Crippen Method
logp	3.934		Crippen Method
mcvol	238.800	ml/mol	McGowan Method
rinpol	2652.00		NIST Webbook
rinpol	2679.00		NIST Webbook
rinpol	2694.00		NIST Webbook
rinpol	2638.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2610.00		NIST Webbook
rinpol	2746.90		NIST Webbook
rinpol	2651.00		NIST Webbook

rinpol	2624.00	NIST Webbook
rinpol	2624.00	NIST Webbook
rinpol	2676.00	NIST Webbook
rinpol	2648.00	NIST Webbook
rinpol	2685.00	NIST Webbook
rinpol	2641.00	NIST Webbook
rinpol	2676.00	NIST Webbook
rinpol	2676.00	NIST Webbook
rinpol	2656.00	NIST Webbook
rinpol	2619.00	NIST Webbook
rinpol	2641.00	NIST Webbook
rinpol	2685.00	NIST Webbook
rinpol	2746.90	NIST Webbook
rinpol	2648.00	NIST Webbook
rinpol	2652.00	NIST Webbook
rinpol	2630.00	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	27.69	kJ/mol	419.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C2955386&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

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