Bromazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 7-bromo-1,3-dihydro-5-(2-pyridinyl)-
	Compedium
	Creosedin
	La xvii
	Lectopam
	Lekotam
	Lexaurin
	Lexilium
	Lexotanil
	Ro 5-3350
	2H-1,4-Benzodiazepin-2-one, 7-bromo-1,3-dihydro-5-(2-pyridyl)-
	7-Bromo-1,3-dihydro-5-(2-pyridyl)-2H-1,4-benzodiazepin-2-one
	7-Bromo-5-(2-pyridyl)-3H-1,4-benzodiazepin-2(1H)-one
	2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-bromo-5-(2-pyridyl)-
	7-Bromo-1,3-dihydro-5-(2-pyridyl)-2H-1,4-benzdiazepin-2-one
	Compendium
	1,3-Dihydro-7-bromo-5-(2-pyridyl)-2H-1,4-benzodiazepin-2-one
	KL-001
	Lexomil
	Lexotan
	Durazanil
	Normoc
	Calmepam
	NSC 140669
Inchi:	InChI=1S/C14H10BrN3O/c15-9-4-5-11-10(7-9)14(17-8-13(19)18-11)12-3-1-2-6-16-12/h1
InchiKey:	VMIYHDSEFNYJSL-UHFFFAOYSA-N
Formula:	C14H10BrN3O
SMILES:	O=C1CN=C(c2ccccn2)c2cc(Br)ccc2N1
Mol. weight [g/mol]:	316.15
CAS:	1812-30-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.86		Crippen Method
logp	2.634		Crippen Method
mcvol	194.450	ml/mol	McGowan Method

rinpol	2626.00	NIST Webbook
rinpol	2591.00	NIST Webbook
rinpol	2601.00	NIST Webbook
rinpol	2613.00	NIST Webbook
rinpol	2633.00	NIST Webbook
rinpol	2626.00	NIST Webbook
rinpol	2626.00	NIST Webbook
rinpol	2613.00	NIST Webbook
rinpol	2613.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1812302&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

rinpol: Non-polar retention indices