Diazepam

Other names:

1-Methyl-5-phenyl-7-chloro-1,3-dihydro-2H-1,4-benzodiazepin-2-one
2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-1-methyl-5-phenyl-
7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one
7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one (diazepam)
7-Chloro-1-methyl-2-oxo-5-phenyl-3H-1,4-benzodiazepine
7-Chloro-1-methyl-5-3H-1,4-benzodiazepin-2(1H)-one
7-Chloro-1-methyl-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one
7-Chloro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one
7-Chloro-1-methyl-5-phenyl-3H-1,4-benzodiazepin-2(1H)-one
Alboral
Aliseum
Alupram
Amiprol
An-Ding
Anlin
Ansiolin
Ansiolisina
Antenex
Apaurin
Apozepam
Armonil
Arzepam
Assival
Atensine
Atilen
Bensedin
Bialzepam
CB 4261
Calmocitene
Calmpose
Cercine
Ceregulart
Condition
D-Pam
Diacepan
Dialag
Dialar
Diapam
Diapax
Diazemuls

Diazepan
Diazetard
Dienpax
Dipam
Dipezona
Domalium
Doval
Drenian
Ducene
Duksen
Duxen
Eridan
Eurosan
Evacalm
Faustan
Freudal
Frustan
Gewacalm
Gihitan
Horizon
Jinpanfan
Kabivitrum
Kiatrium
Kratium
LA 111
LA-III
Lamra
Lembrol
Levium
Liberetas
Mandrozep
Methyldiazepinone
Methyldiazepinone, pharmaceutical
Morosan
NSC-77518
Nellium
Nerozen
Neurolytril
Noan
Novazam
Paceum
Pacitran
Paranten

Paxate
Paxel
Paxum
Placidox 5
Plidan
Pro pam
Q-pam
Quetinil
Quiatril
Quievita
Relaminal
Relanium
Relax
Renborin
Ro 5-2807
Ruhsitus
S.A.R.L.
Saromet
Sedapam
Sedipam
Seduksen
Seduxen
Serenack
Serenamin
Serenzin
Servizepam
Setonil
Sibazon
Simasedan
Sipam
Solis
Sonacon
Stesolid
Stesolin
Tensium
Tensopam
Tranimul
Tranqdyn
Tranquase
Tranquirit
Tranquo-Puren
Tranquo-Tablinen
Umbrium

	Unisedil
	Usempax AP
	Valaxona
	Valeo
	Valiquid
	Valitran
	Valium
	Valrelease
	Vatran
	Vazen
	Velium
	Vival
	Vivol
	Wy 3467
	Zepaxid
	Zipan
Inchi:	InChI=1S/C16H13ClN2O/c1-19-14-8-7-12(17)9-13(14)16(18-10-15(19)20)11-5-3-2-4-6-1
InchiKey:	AAOVKJBEBIDNHE-UHFFFAOYSA-N
Formula:	C16H13ClN2O
SMILES:	CN1C(=O)CN=C(c2ccccc2)c2cc(Cl)ccc21
Mol. weight [g/mol]:	284.74
CAS:	439-14-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.73		Aqueous Solubility Prediction Method
log10ws	-3.75		Estimated Solubility Method
log10ws	-3.75		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	3.154		Crippen Method
mcvol	207.390	ml/mol	McGowan Method
rinpol	2480.00		NIST Webbook
rinpol	2477.00		NIST Webbook
rinpol	2440.00		NIST Webbook
rinpol	2475.00		NIST Webbook
rinpol	2464.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2461.00		NIST Webbook

rinpol	2460.00	NIST Webbook
rinpol	2439.00	NIST Webbook
rinpol	2426.00	NIST Webbook
rinpol	2440.00	NIST Webbook
rinpol	2477.00	NIST Webbook
rinpol	2485.00	NIST Webbook
rinpol	2407.00	NIST Webbook
rinpol	2525.80	NIST Webbook
rinpol	2460.00	NIST Webbook
rinpol	2404.00	NIST Webbook
rinpol	2407.00	NIST Webbook
rinpol	2404.00	NIST Webbook
rinpol	2405.00	NIST Webbook
rinpol	2436.00	NIST Webbook
rinpol	2425.00	NIST Webbook
rinpol	2409.00	NIST Webbook
rinpol	2439.00	NIST Webbook
rinpol	2474.00	NIST Webbook
rinpol	2425.00	NIST Webbook
rinpol	2425.00	NIST Webbook
rinpol	2471.00	NIST Webbook
rinpol	2477.00	NIST Webbook
rinpol	2448.00	NIST Webbook
rinpol	2404.00	NIST Webbook
rinpol	2407.00	NIST Webbook
rinpol	2415.00	NIST Webbook
rinpol	2405.00	NIST Webbook
rinpol	2405.00	NIST Webbook
rinpol	2430.00	NIST Webbook
rinpol	2425.00	NIST Webbook
rinpol	2434.00	NIST Webbook
rinpol	2408.00	NIST Webbook
rinpol	2408.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2415.00	NIST Webbook
rinpol	2417.00	NIST Webbook
rinpol	2408.00	NIST Webbook
rinpol	2410.00	NIST Webbook
rinpol	2419.00	NIST Webbook
rinpol	2425.00	NIST Webbook
rinpol	2436.00	NIST Webbook

rinpol	2410.00		NIST Webbook
rinpol	2425.00		NIST Webbook
rinpol	2525.80		NIST Webbook
rinpol	2405.00		NIST Webbook
rinpol	2440.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2417.00		NIST Webbook
rinpol	2436.00		NIST Webbook
rinpol	2425.00		NIST Webbook
rinpol	2404.00		NIST Webbook
rinpol	2439.00		NIST Webbook
rinpol	2461.00		NIST Webbook
tf	402.00	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	24.70	kJ/mol	404.80	NIST Webbook
hfust	25.49	kJ/mol	403.60	NIST Webbook

Sources

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

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C439145&Units=SI

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

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

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