Lorazepam

Other names:

(.+/-.)-Lorazepam
2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-
2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(o-chlorophenyl)-1,3-dihydro-3-hydroxy-
7-Chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one
7-Chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one
((+)lorazepam)
7-Chloro-5-(2-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one
((Â±)lorazepam)
7-Chloro-5-(2-chlorophenyl)-3-hydroxy-1H-1,4-benzodiazepin-2(3H)-one
7-Chloro-5-(o-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one
Almazine
Anxiedin
Anxira
Anzepam
Aplacasse
Apo-Lorazepam
Aripax
Ativan
Azurogen
Bonatranquan
Bonton
Delormetazepam
Demethyllormetazepam
Duralozam
Efasedan
Emotival
Equitam
Kalmalin
Larpose
Laubeel
Lorabenz
Loram
Lorapam
Lorat
Lorax
Lorazene
Lorazep
Lorazin
Lorenin
Loridem
Lorsedal
Lorsilan

	Lozepam
	Merlit
	NSC 289758
	Nervistop L
	Norlormetazepam
	Novhepar
	Orfidal
	Pro dorm
	Psicopax
	Punktyl
	Quait
	Renaquil
	Rocosgen
	Securit
	Sedatival
	Sedazin
	Sedizepan
	Sidenar
	Silence
	Somagerol
	Stapam
	Tavor
	Temesta
	Titus
	Tranqipam
	Trapax
	Upan
	Wy 4036
	Wypax
	o-Chlorooxazepam
	o-Chloroxazepam
Inchi:	InChI=1S/C15H10Cl2N2O2/c16-8-5-6-12-10(7-8)13(19-15(21)14(20)18-12)9-3-1-2-4-11(
InchiKey:	DIWRORZWFLOCLC-UHFFFAOYSA-N
Formula:	C15H11Cl2N2O2
SMILES:	OC1=Nc2ccc(Cl)cc2C(c2ccccc2Cl)=NC1O
Mol. weight [g/mol]:	322.17
CAS:	846-49-1

Physical Properties

Property code	Value	Unit	Source

gf	284.62	kJ/mol	Joback Method
hf	44.82	kJ/mol	Joback Method
hfus	43.97	kJ/mol	Joback Method
hvap	112.23	kJ/mol	Joback Method
log10ws	-1.77		Aqueous Solubility Prediction Method
log10ws	-3.60		Estimated Solubility Method
logp	3.751		Crippen Method
mcvol	211.410	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2402.00		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	2492.80		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2423.00		NIST Webbook
rinpol	2442.00		NIST Webbook
rinpol	2391.00		NIST Webbook
rinpol	2411.00		NIST Webbook
rinpol	2423.00		NIST Webbook
rinpol	2448.00		NIST Webbook
rinpol	2423.00		NIST Webbook
rinpol	2384.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2442.00		NIST Webbook
rinpol	2440.00		NIST Webbook
rinpol	2411.00		NIST Webbook
rinpol	2399.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2492.80		NIST Webbook
rinpol	2426.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
rinpol	2430.00		NIST Webbook
rinpol	2395.00		NIST Webbook
rinpol	2391.00		NIST Webbook
tb	1001.08	K	Joback Method
tc	1250.13	K	Joback Method
tf	439.75	K	Aqueous Solubility Prediction Method

vc	0.806	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.98	J/mol×K	1001.08	Joback Method
cpg	631.26	J/mol×K	1042.59	Joback Method
cpg	636.19	J/mol×K	1084.10	Joback Method
cpg	639.78	J/mol×K	1125.61	Joback Method
cpg	642.07	J/mol×K	1167.12	Joback Method
cpg	643.08	J/mol×K	1208.62	Joback Method
cpg	642.83	J/mol×K	1250.13	Joback Method
hfust	75.20	kJ/mol	453.20	NIST Webbook
hfust	92.57	kJ/mol	446.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Chlordiazepoxide, Diazepam, and Lorazepam in Ethanol + Water Mixtures at 303.2 K:	https://www.doi.org/10.1021/je900200k
Solubility of 7-Chloro-2-methylamino-5-phenyl-3H-1,4-benzodiazepine-4-oxide, 7-Chloro-1,3-dihydro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one, and 7-Chloro-5-(2-chlorophenyl)-3-hydroxy-1,3-dihydro-1,4-benzodiazepin-2-one in (Propane-1,2-diol + Water) at a Temperature of 303.2 K:	https://www.doi.org/10.1021/je900451d
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C846491&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume