Clonazepam

Other names: 1,3-Dihydro-7-nitro-5-(2-chlorophenyl)-2H-1,4.benzodiazepin-2-one
2H-1,4-Benzodiazepin-2-one, 5-(2-chlorophenyl)-1,3-dihydro-7-nitro-
2H-1,4-Benzodiazepin-2-one, 5-(o-chlorophenyl)-1,3-dihydro-7-nitro-
5-(2-Chlorophenyl)-1,3-dihydro-7-nitro-2H-1,4-benzodiazepin-2-one
5-(o-Chlorophenyl)-1,3-dihydro-7-nitro-2H-1,4-benzodiazepin-2-one
7-Nitro-5-(2-chlorophenyl)-3H-1,4-benzodiazepin-2(1H)-one
Antelepsin
Chlonazepam
Cloazepam
Clonex
Clonopin
Iktorivil
Kenoket
Klonopin
Landsen
Lonazep
NSC 179913
Paxam
Rivotril
Ro 4-8180
Ro 5-4023

Inchi: InChI=1S/C15H10ClN3O3/c16-12-4-2-1-3-10(12)15-11-7-9(19(21)22)5-6-13(11)18-14(20

InchiKey: DGBIGWXXNGSACT-UHFFFAOYSA-N

Formula: C15H10ClN3O3

SMILES: O=C1CN=C(c2ccccc2Cl)c2cc([N+](=O)[O-])ccc2N1

Mol. weight [g/mol]: 315.71

CAS: 1622-61-3

Physical Properties

Property code	Value	Unit	Source
gf	441.46	kJ/mol	Joback Method
hf	157.43	kJ/mol	Joback Method
hfus	45.01	kJ/mol	Joback Method
hvap	95.23	kJ/mol	Joback Method
log10ws	-3.50		Estimated Solubility Method

log10ws	-3.82		Aqueous Solubility Prediction Method
logp	3.038		Crippen Method
mcvol	210.720	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	2934.60		NIST Webbook
rinpol	2885.00		NIST Webbook
rinpol	2833.00		NIST Webbook
rinpol	2813.00		NIST Webbook
rinpol	2885.00		NIST Webbook
rinpol	2814.00		NIST Webbook
rinpol	2879.00		NIST Webbook
rinpol	2833.00		NIST Webbook
rinpol	2934.60		NIST Webbook
rinpol	2878.00		NIST Webbook
rinpol	2856.00		NIST Webbook
rinpol	2832.00		NIST Webbook
rinpol	2860.00		NIST Webbook
rinpol	2803.00		NIST Webbook
rinpol	2806.00		NIST Webbook
rinpol	2860.00		NIST Webbook
rinpol	2885.00		NIST Webbook
rinpol	2833.00		NIST Webbook
tb	994.33	K	Joback Method
tc	1297.93	K	Joback Method
tf	510.65	K	Aqueous Solubility Prediction Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.78	J/mol×K	994.33	Joback Method
cpg	636.00	J/mol×K	1044.93	Joback Method
cpg	641.99	J/mol×K	1095.53	Joback Method
cpg	645.75	J/mol×K	1146.13	Joback Method
cpg	647.30	J/mol×K	1196.73	Joback Method
cpg	646.65	J/mol×K	1247.33	Joback Method
cpg	643.80	J/mol×K	1297.93	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Solubility of Clonazepam, Diazepam, Lamotrigine, and Phenobarbital in N-Methyl-2-pyrrolidone + Water Mixtures at 298.2 K:	https://www.doi.org/10.1021/je9000153
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1622613&Units=SI
Solubility of Lamotrigine, Diazepam, Clonazepam, and Phenobarbital in Propylene Glycol + Water Mixtures at 298.15 K:	https://www.doi.org/10.1021/je800931z
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Clonazepam and Diazepam in Polyethylene Glycol 200, Propylene Glycol, N-Methyl Pyrrolidone, Ethanol, and Water at (298.2 to 313.2) K and in Binary and Ternary Mixtures of Polyethylene Glycol 200, Propylene Glycol, and Water at 298.2 K:	https://www.doi.org/10.1021/je3009842
Solubility of Lamotrigine, Diazepam, and Clonazepam in Ethanol + Water Mixtures at 298.2 K:	https://www.doi.org/10.1021/je8007827
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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