Oxazepam

Other names:

(.+/-.)-Oxazepam
(RS)-Oxazepam
2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-3-hydroxy-5-phenyl-
7-Chloro-1,3-dihydro-3-hydroxy-5-phenyl-2H-1,4-benzodiazepin-2-one
7-Chloro-1,3-dihydro-3-hydroxy-5-phenyl-2H-1,4-benzodiazepine-2-one
7-Chloro-1,3-dihydroxy-5-phenyl-2H-1,4-benzodiazepin-2-one ((±)-oxazepam)
7-Chloro-1,3-dihydroxy-5-phenyl-2H-1,4-benzodiazepin-2-one ((Â±)-oxazepam)
7-Chloro-3-hydroxy-5-phenyl-1,3-dihydro-2H-1,4-benzodiazepin-2-one
7-Chloro-3-hydroxy-5-phenyl-1,3-dihydro-benzo[e][1,4]diazepin-2-one
7-chloro-3-hydroxy-5-phenyl-1,3-dihydro-1,4-benzodiazepin-2-one
Adumbran
Ansiolisina
Ansioxacepam
Anxiolit
Aplakil
Astress
Azutranquil
Bonare
CB 8092
Camazepam-metabolite
Clorazepate-metabolite
Diazepam-metabolite
Drimuel
Droxacepam
Durazepam
Enidrel
Hi-Long
Isodin
Ketazolam-metabolite
Lederpam
Limbial
Murelax
Nesontil
Noctazepam
Nortemazepam
Notaral
Nozepam
Oxa-puren
Oxanid
Oxozepam

Pacienx
Praxiten
Propax
Psicopax
Psiquiwas
QUEN
Quilibrex
Ro 5-6789
Rondar
Sedigoa
Serax
Serenal
Serenid
Serenid-D
Serepax
Seresta
Serpax
Sigacalm
Sobril
Tacepam
Tarchomin
Tazepam
Temazepam-metabolite
Tranquo-buscopan-wirkstoff
Uskan
Vaben
Wy-3498
Wy-3498 stic
Z10-TR
Zaxopam

Inchi: InChI=1S/C15H11ClN2O2/c16-10-6-7-12-11(8-10)13(9-4-2-1-3-5-9)18-15(20)14(19)17-1

InchiKey: ADIMAYPTOBDMTL-UHFFFAOYSA-N

Formula: C15H12ClN2O2

SMILES: O=C1Nc2ccc(Cl)cc2C(c2ccccc2)=NC1O

Mol. weight [g/mol]: 287.72

CAS: 604-75-1

Physical Properties

Property code	Value	Unit	Source

gf	271.01	kJ/mol	Joback Method
hf	7.09	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	94.35	kJ/mol	Joback Method
log10ws	-3.95		Aqueous Solubility Prediction Method
log10ws	-3.95		Estimated Solubility Method
logp	2.448		Crippen Method
mcvol	199.170	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2323.00		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2385.00		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	2320.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2386.00		NIST Webbook
rinpol	2373.00		NIST Webbook
rinpol	2374.00		NIST Webbook
rinpol	2336.00		NIST Webbook
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
rinpol	2354.00		NIST Webbook
rinpol	2293.00		NIST Webbook
rinpol	2294.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
rinpol	2336.00		NIST Webbook
rinpol	2310.00		NIST Webbook
rinpol	2336.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2335.00		NIST Webbook
rinpol	2350.00		NIST Webbook
rinpol	2370.00		NIST Webbook

rinpol	2336.00		NIST Webbook
tb	925.02	K	Joback Method
tc	1190.00	K	Joback Method
tf	478.45	K	Aqueous Solubility Prediction Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.70	J/mol×K	1101.68	Joback Method
cpg	627.83	J/mol×K	1145.84	Joback Method
cpg	594.96	J/mol×K	925.02	Joback Method
cpg	604.98	J/mol×K	969.18	Joback Method
cpg	613.28	J/mol×K	1013.35	Joback Method
cpg	619.85	J/mol×K	1057.51	Joback Method
cpg	629.23	J/mol×K	1190.00	Joback Method
hfust	86.40	kJ/mol	478.80	NIST Webbook
hfust	84.11	kJ/mol	467.50	NIST Webbook

Sources

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=C604751&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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