Nitrazepam

Other names:

1,3-Dihydro-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one
1,3-Dihydro-7-nitro-5-phenyl-2H-1,4-benzodiazepine-2-one
2,3-Dihydro-7-nitro-5-phenyl-1H-1,4-benzodiazepin-2-one
2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-nitro-5-phenyl-
7-Nitro-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one
7-Nitro-5-phenyl-2,3-dihydro-1H-1,4-benzodiazepin-2-one
7-nitro-5-phenyl-1,3-dihydro-1,4-benzodiazepin-2-one
Apodorm
Benzalin
Calsmin
Cerson
Dormicum
Dormin-5
Dumolid
Eatan
Epibenzalin
Epinelbon
Eunoctin
Eunoktin
Hipnax
Hipsal
Imeson
Imesont
Insomin
Ipersed
LA 1
Magadon
Megadon
Mogadan
Mogadon
Mogadone
N-Desmethylnimetazepam
NSC-58775
Nelbon
Nelmat
Neozepam
Neuchlonic
Nitrados
Nitravet
Nitrenpax

Noctesed
Paxisyn
Pelson
Radedorm
Relact
Remnos
Ro 4-5360
Ro 5-3059
S 2000
Somitran
Somnased
Somnibel
Somnite
Sonebon
Sonnolin
Surem
Trazenin
Unisomnia

Inchi: InChI=1S/C15H11N3O3/c19-14-9-16-15(10-4-2-1-3-5-10)12-8-11(18(20)21)6-7-13(12)17

InchiKey: KJONHKAYOJNZEC-UHFFFAOYSA-N

Formula: C15H11N3O3

SMILES: O=C1CN=C(c2ccccc2)c2cc([N+](=O)[O-])ccc2N1

Mol. weight [g/mol]: 281.27

CAS: 146-22-5

Physical Properties

Property code	Value	Unit	Source
gf	463.02	kJ/mol	Joback Method
hf	184.64	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	90.19	kJ/mol	Joback Method
log10ws	-3.79		Aqueous Solubility Prediction Method
log10ws	-3.80		Estimated Solubility Method
logp	2.384		Crippen Method
mcvol	198.480	ml/mol	McGowan Method
pc	3384.14	kPa	Joback Method
rinpol	2728.00		NIST Webbook
rinpol	2740.00		NIST Webbook

rinpol	2775.00	NIST Webbook
rinpol	2724.00	NIST Webbook
rinpol	2740.00	NIST Webbook
rinpol	2785.00	NIST Webbook
rinpol	2765.00	NIST Webbook
rinpol	2849.90	NIST Webbook
rinpol	2780.00	NIST Webbook
rinpol	2795.00	NIST Webbook
rinpol	2740.00	NIST Webbook
rinpol	2765.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2780.00	NIST Webbook
rinpol	2790.00	NIST Webbook
rinpol	2790.00	NIST Webbook
rinpol	2795.00	NIST Webbook
rinpol	2800.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2770.00	NIST Webbook
rinpol	2800.00	NIST Webbook
rinpol	2820.00	NIST Webbook
rinpol	2772.00	NIST Webbook
rinpol	2720.00	NIST Webbook
rinpol	2777.00	NIST Webbook
rinpol	2778.00	NIST Webbook
rinpol	2780.00	NIST Webbook
rinpol	2780.00	NIST Webbook
rinpol	2782.00	NIST Webbook
rinpol	2788.00	NIST Webbook
rinpol	2790.00	NIST Webbook
rinpol	2794.00	NIST Webbook
rinpol	2800.00	NIST Webbook
rinpol	2780.00	NIST Webbook
rinpol	2744.00	NIST Webbook
rinpol	2720.00	NIST Webbook
rinpol	2820.00	NIST Webbook
rinpol	2750.00	NIST Webbook
rinpol	2750.00	NIST Webbook
rinpol	2755.00	NIST Webbook
rinpol	2755.00	NIST Webbook

rinpol	2755.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2730.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2728.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2775.00		NIST Webbook
rinpol	2746.00		NIST Webbook
tb	951.92	K	Joback Method
tc	1255.27	K	Joback Method
tf	753.51	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.59	J/mol×K	951.92	Joback Method
cpg	624.04	J/mol×K	1002.48	Joback Method
cpg	632.26	J/mol×K	1053.04	Joback Method
cpg	638.27	J/mol×K	1103.59	Joback Method
cpg	642.10	J/mol×K	1154.15	Joback Method
cpg	643.75	J/mol×K	1204.71	Joback Method
cpg	643.27	J/mol×K	1255.27	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C146225&Units=SI

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

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

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

Latest version available from:
https://www.chemeo.com/cid/38-801-0/Nitrazepam.pdf
Generated by Cheméo on 2024-04-29 20:17:34.797887525 +0000 UTC m=+16711103.718464841.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.