Pemoline

Other names:

4(5H)-Oxazolone, 2-amino-5-phenyl-
Azoksodon
Azoxodon
Azoxodone
Centramin
Dantromin
Deltamin
Hyton
Kethamed
LA 956
Okodon
Pemolin
Pheniminooxazolidinone
Phenoxazole
Phenylisohydantoin
Phenylpseudohydantoin
Pioxol
Pondex
PIO
Ronyl
Sistra
Stimul
Stimulol
Tradon
Tradone
Yh 1
A 13397
Abbott 13397
Betanamin
C- 293
Constimol
Cylert
Deltamine
Endolin
Fenoxazol
Fio
Fwh-352
H 310
Juston-Wirkstoff
Myamin

	Nitan
	NPL 1
	Phenalone
	Phenilone
	Pn/135
	Pomoline
	PT 360
	Sigmadyn
	Sistral
	Sofro
	Volital
	Volitol
	2-Imino-5-phenyl-4-oxazolidinone
	4-Oxazolidinone, 2-imino-5-phenyl-
	5-Phenyl-2-imino-4-oxazolidinone
	2-Amino-5-phenyl-4(5H)-oxazolone
	CS 293
	H 3104
	Notair
	Pemolina
	5-Phenyl-2-imino-4-oxooxazolidine
	Hyton asa
	NSC-25159
	Senior
	2-Imino-4-keto-5-phenyltetrahydrooxazole
	2-Oxazolin-4-one, 2-amino-5-phenyl-
Inchi:	InChI=1S/C9H8N2O2/c10-9-11-8(12)7(13-9)6-4-2-1-3-5-6/h1-5,7H,(H2,10,11,12)
InchiKey:	NRNCYVBFPDDJNE-UHFFFAOYSA-N
Formula:	C9H8N2O2
SMILES:	NC1=NC(=O)C(c2ccccc2)O1
Mol. weight [g/mol]:	176.17
CAS:	2152-34-3

Physical Properties

Property code	Value	Unit	Source
gf	168.71	kJ/mol	Joback Method
hf	-50.71	kJ/mol	Joback Method
hfus	25.70	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method

log10ws	-1.50		Crippen Method
logp	0.599		Crippen Method
mcvol	126.150	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	672.42	K	Joback Method
tc	949.61	K	Joback Method
tf	491.38	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.99	J/mol×K	672.42	Joback Method
cpg	363.77	J/mol×K	718.62	Joback Method
cpg	377.17	J/mol×K	764.82	Joback Method
cpg	389.17	J/mol×K	811.01	Joback Method
cpg	399.76	J/mol×K	857.21	Joback Method
cpg	408.92	J/mol×K	903.41	Joback Method
cpg	416.62	J/mol×K	949.61	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2152343&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
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