

Clonidine

Other names:

1H-Imidazol-2-amine, N-(2,6-dichlorophenyl)-4,5-dihydro-
2-Imidazoline, 2-(2,6-dichloroanilino)-
734571A
Benzenamine, 2,6-dichloro-N-2-imidazolidinylidene-
Clonidin
2-(2,6-Dichlorophenylamino)-2-imidazoline
2-[(2,6-Dichlorophenyl)imino]imidazolidine
Catapres-TTS
2-[(2,6-Dichlorophenyl)imino]imidazoline
ST-155-BS
2-(2,6-Dichloroanilino)-2-imidazoline
M 5041T
SKF 34427

Inchi:

InChI=1S/C9H9Cl2N3/c10-6-2-1-3-7(11)8(6)14-9-12-4-5-13-9/h1-3H,4-5H2,(H2,12,13,14)

InchiKey:

GJSURZIOUXUGAL-UHFFFAOYSA-N

Formula:

C9H9Cl2N3

SMILES:

Clc1cccc(Cl)c1N=C1NCCN1

Mol. weight [g/mol]:

230.09

CAS:

4205-90-7

Physical Properties

Property code	Value	Unit	Source
hf	150.49	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.174		Crippen Method
mcvol	153.170	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
rinpol	2023.00		NIST Webbook
rinpol	2023.00		NIST Webbook
rinpol	2065.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	713.03	K	Joback Method
tc	987.82	K	Joback Method

Sources

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=C4205907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation 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

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