1-PHENYLPYRAZOLIDIN-3-ONE

Other names:	Fenidon
	Phenidone
	1-Phenyl-3-oxopyrazolidine
	1-Phenyl-3-pyrazolidinone
	1-Phenyl-3-pyrazolidone
	1-Phenylpyrazolid-3-one
	2-Pyrazolin-3-ol, 1-phenyl-
	1-P-3-P
	1-Phenyl-pyrazolidin-3-one
Inchi:	InChI=1S/C9H10N2O/c12-9-6-7-11(10-9)8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,12)
InchiKey:	CMCWWLVWPDLCRM-UHFFFAOYSA-N
Formula:	C9H10N2O
SMILES:	O=C1CCN(c2ccccc2)N1
Mol. weight [g/mol]:	162.19

Physical Properties

Property code	Value	Unit	Source
logp	0.928		Crippen Method
mcvol	124.580	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	84.30	kJ/mol	337.50	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C92433&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hsubt: Enthalpy of sublimation at a given temperature

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume