

3H-Pyrazol-3-one, 2,4-dihydro-2-methyl-5-phenyl-

Inchi: InChI=1S/C10H10N2O/c1-12-10(13)7-9(11-12)8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey: NIXIJMXBXHWPEK-UHFFFAOYSA-N
Formula: C10H10N2O
SMILES: CN1N=C(c2ccccc2)CC1=O
Mol. weight [g/mol]: 174.20
CAS: 41927-50-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.61		Crippen Method
logp	1.253		Crippen Method
mcpvol	134.370	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	508.20	K	9.10	NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C41927508&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tbrp: Boiling point at reduced pressure

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