4-ISOPROPYL-2,3-DIMETHYL-1-PHENYL-3-PYRAZ

Other names: 3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimethyl-4-(1-methylethyl)-2-phenyl-
Antipyrine, 4-isopropyl-
2,3-Dimethyl-4-isopropyl-1-phenyl-3H-pyrazolin-5-one
Isopropylantipyrin
Isopropylantipyrine
4-Isopropylantipyrine
4-Isopropyl-2,3-dimethyl-1-phenyl-3-pyrazolin-5-one
Isopropylphenazone
Larodon
1-Phenyl-2,3-dimethyl-4-isopropyl-3-pyrazolin-5-one
1-Phenyl-2,3-dimethyl-4-isopropylpyrazol-5-one
3-Pyrazolin-5-one, 2,3-dimethyl-4-isopropyl-1-phenyl-
3-Pyrazolin-5-one, 4-isopropyl-2,3-dimethyl-1-phenyl-
Isopropyrine
4-Isopropylphenazone
Budirol
Causyth
Cibalgina
Eufibron
Isopropchin

Inchi: InChI=1S/C14H18N2O/c1-10(2)13-11(3)15(4)16(14(13)17)12-8-6-5-7-9-12/h5-10H,1-4H3

InchiKey: PXWLVJLKJGVOKE-UHFFFAOYSA-N

Formula: C14H18N2O

SMILES: Cc1c(C(C)C)c(=O)n(-c2ccccc2)n1C

Mol. weight [g/mol]: 230.31

Physical Properties

Property code	Value	Unit	Source
ie	7.67	eV	Cheméo Relay (1.0)
log10ws	-1.33		Cheméo Relay (1.0)
logp	2.608		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
tf	388.15	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C479925
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

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point