

4-Methyl-2-pentanone, 2,4-dinitrophenyl-hydrazone

Other names: 2-Pentanone, 4-methyl-, (2,4-dinitrophenyl)hydrazone

Inchi: InChI=1S/C12H16N4O4/c1-8(2)6-9(3)13-14-11-5-4-10(15(17)18)7-12(11)16(19)20/h4-5,7,9,11,12,14,15,17,18,20

InchiKey: UNLVZDNGQXFBAY-UKTHLTGXSA-N

Formula: C12H16N4O4

SMILES: CC(CC(C)C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]

Mol. weight [g/mol]: 280.28

CAS: 1655-42-1

Physical Properties

Property code	Value	Unit	Source
hf	21.68	kJ/mol	Joback Method
hvap	88.53	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.337		Crippen Method
mcvol	206.680	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2468.00		NIST Webbook
rinpol	2468.00		NIST Webbook
tb	940.57	K	Joback Method
tc	1200.92	K	Joback Method

Sources

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=C1655421&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

hf:	Enthalpy of formation at standard conditions
hvac:	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
rinqol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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