

3,3-Dimethyl-2-butanone, 2,4-dinitrophenyl hydrazone

Other names:	2-Butanone, 3,3-dimethyl-, (2,4-dinitrophenyl)hydrazone
Inchi:	InChI=1S/C12H16N4O4/c1-8(12(2,3)4)13-14-10-6-5-9(15(17)18)7-11(10)16(19)20/h5-7,1
InchiKey:	OMNJXFSXEYYSRY-UHFFFAOYSA-N
Formula:	C12H16N4O4
SMILES:	CC(=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-])C(C)(C)C
Mol. weight [g/mol]:	280.28
CAS:	964-53-4

Physical Properties

Property code	Value	Unit	Source
hf	18.21	kJ/mol	Joback Method
hvap	87.62	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.337		Crippen Method
mcvol	206.680	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2433.00		NIST Webbook
tb	937.78	K	Joback Method
tc	1205.87	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C964534&Units=SI

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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