2-Butanone, 3-methyl-, (2,4-dinitrophenyl)hydrazone

Other names: 3-Methyl-2-butanone 2,4-dinitrophenylhydrazone
Methyl isopropyl ketone-dnph

Inchi: InChI=1S/C11H14N4O4/c1-7(2)8(3)12-13-10-5-4-9(14(16)17)6-11(10)15(18)19/h4-7,13H

InchiKey: WXKQSBKURZFLTH-UHFFFAOYSA-N

Formula: C11H14N4O4

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

Mol. weight [g/mol]: 266.25

CAS: 3077-97-2

Physical Properties

Property code	Value	Unit	Source
hf	42.32	kJ/mol	Joback Method
hvap	86.30	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.947		Crippen Method
mcvol	192.590	ml/mol	McGowan Method
pc	2431.44	kPa	Joback Method
rinpol	2386.00		NIST Webbook
tb	917.69	K	Joback Method
tc	1182.71	K	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C3077972&Units=SI

Legend

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