

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

Other names:

Isovaleraldehyde, (2,4-dinitrophenyl)hydrazone

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

Isovaleraldehyde dnp

Isovaleraldehyde, 2,4-dinitrophenylhydrazone

Inchi:

InChI=1S/C11H14N4O4/c1-8(2)5-6-12-13-10-4-3-9(14(16)17)7-11(10)15(18)19/h3-4,6-8,

InchiKey:

MCWYOPWJODIZJK-UHFFFAOYSA-N

Formula:

C11H14N4O4

SMILES:

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

Mol. weight [g/mol]:

266.25

CAS:

2256-01-1

Physical Properties

Property code	Value	Unit	Source
hf	52.11	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.947		Crippen Method
mcvol	192.590	ml/mol	McGowan Method
pc	2419.50	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	917.81	K	Joback Method
tc	1179.23	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=C2256011&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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