2,4-dinitrophenylhydrazone 2-methyl-1-hexen-5-one

Inchi: InChI=1S/C13H16N4O4/c1-9(2)4-5-10(3)14-15-12-7-6-11(16(18)19)8-13(12)17(20)21/h6

InchiKey: XAMZCDKGQBWOPL-UHFFFAOYSA-N

Formula: C13H16N4O4

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

Mol. weight [g/mol]: 292.29

Physical Properties

Property code	Value	Unit	Source
hf	121.96	kJ/mol	Joback Method
hvap	90.55	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	3.647		Crippen Method
mcvol	216.470	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	2610.00		NIST Webbook
rinpol	2610.00		NIST Webbook
tb	960.45	K	Joback Method
tc	1220.00	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R139654&Units=SI

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

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