2,4-dinitrophenylhydrazone 2-methyl-5-hexanone

Inchi: InChI=1S/C13H18N4O4/c1-9(2)4-5-10(3)14-15-12-7-6-11(16(18)19)8-13(12)17(20)21/h6

InchiKey: RBVLNDINMWKLOR-GXDHUFHOSA-N

Formula: C13H18N4O4

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

Mol. weight [g/mol]: 294.31

Physical Properties

Property code	Value	Unit	Source
hf	1.04	kJ/mol	Joback Method
hvap	90.76	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.727		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2584.00		NIST Webbook
tb	963.45	K	Joback Method
tc	1219.90	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R139689&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

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

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