

2,4-Dinitrophenylhydrazone of 6-methyl-5-heptenone-2

Other names:	5-Hepten-2-one, 6-methyl-, (2,4-dinitrophenyl)hydrazone
Inchi:	InChI=1S/C14H18N4O4/c1-10(2)5-4-6-11(3)15-16-13-8-7-12(17(19)20)9-14(13)18(21)22
InchiKey:	KXKSTFJRCXDCBU-RVDMUPIBSA-N
Formula:	C14H18N4O4
SMILES:	CC(C)=CCCC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	306.32
CAS:	6147-43-9

Physical Properties

Property code	Value	Unit	Source
hf	93.11	kJ/mol	Joback Method
hvap	93.41	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.037		Crippen Method
mcvol	230.560	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2706.00		NIST Webbook
rinpol	2706.00		NIST Webbook
tb	990.81	K	Joback Method
tc	1250.38	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=C6147439&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

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