5-Hexen-2-one-p-nitro-phenyl hydrazone

Inchi: InChI=1S/C12H15N3O2/c1-3-4-5-10(2)13-14-11-6-8-12(9-7-11)15(16)17/h3,6-9,14H,1,4-
InchiKey: AZWOVWJAEWTVGJ-JLHYYAGUSA-N
Formula: C12H15N3O2
SMILES: C=CCCC(C)=NNc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 233.27
CAS: 116435-43-9

Physical Properties

Property code	Value	Unit	Source
hf	174.62	kJ/mol	Joback Method
hvap	71.00	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.349		Crippen Method
mcvol	184.960	ml/mol	McGowan Method
pc	2295.91	kPa	Joback Method
tb	780.87	K	Joback Method
tc	1025.07	K	Joback Method

Sources

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=C116435439&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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