

2-Hexenal, 2,4-dinitrophenyl hydrazone

Inchi: InChI=1S/C12H14N4O4/c1-2-3-4-5-8-13-14-11-7-6-10(15(17)18)9-12(11)16(19)20/h4-9,
InchiKey: RRKSQJQLBKPGCP-VDXACTLNSA-N
Formula: C12H14N4O4
SMILES: CCCC=CC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 278.26
CAS: 1560-68-5

Physical Properties

Property code	Value	Unit	Source
hf	153.97	kJ/mol	Joback Method
hvap	88.80	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.257		Crippen Method
mcvol	202.380	ml/mol	McGowan Method
pc	2300.32	kPa	Joback Method
tb	945.29	K	Joback Method
tc	1206.22	K	Joback Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1560685&Units=SI>
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>

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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