

2-Ethylhexenal-2, 2,4-dinitrophenyl hydrazone

Inchi: InChI=1S/C14H18N4O4/c1-3-5-6-11(4-2)10-15-16-13-8-7-12(17(19)20)9-14(13)18(21)22
InchiKey: XLEDIUUKLRZIKQG-FDCMAIFOSA-N
Formula: C14H18N4O4
SMILES: CCCC=C(C=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-])CC
Mol. weight [g/mol]: 306.32
CAS: 10324-64-8

Physical Properties

Property code	Value	Unit	Source
hf	102.90	kJ/mol	Joback Method
hvap	93.33	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.037		Crippen Method
mcvol	230.560	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
tb	990.93	K	Joback Method
tc	1247.64	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=C10324648&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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