

4-Heptanone, (2,4-dinitrophenyl)hydrazone

Inchi: InChI=1S/C13H18N4O4/c1-3-5-10(6-4-2)14-15-12-8-7-11(16(18)19)9-13(12)17(20)21/h7
InchiKey: PUGYZTOHWZGYEY-UHFFFAOYSA-N
Formula: C13H18N4O4
SMILES: CCCC(CCC)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 294.31
CAS: 1655-41-0

Physical Properties

Property code	Value	Unit	Source
hf	6.32	kJ/mol	Joback Method
hvap	91.14	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	3.871		Crippen Method
mcvol	220.770	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	963.89	K	Joback Method
tc	1216.84	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1655410&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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