

3-Methylcyclopentanone 2,4-dinitrophenylhydrazone

Inchi: InChI=1S/C12H14N4O4/c1-8-2-3-9(6-8)13-14-11-5-4-10(15(17)18)7-12(11)16(19)20/h4-10
InchiKey: VFFFGFXWGACQOI-LCYFTJDESA-N
Formula: C12H14N4O4
SMILES: CC1CCC(=NNc2ccc([N+](=O)[O-])cc2[N+](=O)[O-])C1
Mol. weight [g/mol]: 278.26

Physical Properties

Property code	Value	Unit	Source
hf	56.04	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.091		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	958.89	K	Joback Method
tc	1235.68	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=B6000700&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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