

2-((E)-[(2,4-dinitrophenyl)hydrazono]methyl)benzoic acid

InChI: InChI=1S/C14H10N4O6/c19-14(20)11-4-2-1-3-9(11)8-15-16-12-6-5-10(17(21)22)7-13(12)
InChIKey: NJIWCXYRLFQRKD-OVCLIPMQSA-N
Formula: C14H10N4O6
SMILES: O=C(O)c1ccccc1C=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 330.25
CAS: 39101-64-9

Physical Properties

Property code	Value	Unit	Source
hf	-44.28	kJ/mol	Joback Method
hvap	119.65	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	2.647		Crippen Method
mcvol	218.540	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	1164.60	K	Joback Method
tc	1438.89	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=C39101649&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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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