

Propanal, 2,2-dimethyl-, (2,4-dinitrophenyl)hydrazone

Inchi: InChI=1S/C11H14N4O4/c1-11(2,3)7-12-13-9-5-4-8(14(16)17)6-10(9)15(18)19/h4-7,13H,
InchiKey: ORILNCDDCQWASM-UHFFFAOYSA-N
Formula: C11H14N4O4
SMILES: CC(C)(C)C=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 266.25
CAS: 13608-36-1

Physical Properties

Property code	Value	Unit	Source
hf	48.64	kJ/mol	Joback Method
hvap	85.32	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	2.947		Crippen Method
mcvol	192.590	ml/mol	McGowan Method
pc	2445.89	kPa	Joback Method
rinpol	2327.00		NIST Webbook
rinpol	2327.00		NIST Webbook
tb	915.02	K	Joback Method
tc	1184.63	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13608361&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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