

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

Inchi:	InChI=1S/C9H8N4O4/c1-2-5-10-11-8-4-3-7(12(14)15)6-9(8)13(16)17/h2-6,11H,1H2
InchiKey:	JJPZHGIIYUVFTGG-UHFFFAOYSA-N
Formula:	C9H8N4O4
SMILES:	<chem>C=CC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]</chem>
Mol. weight [g/mol]:	236.18
CAS:	888-54-0

Physical Properties

Property code	Value	Unit	Source
hf	224.10	kJ/mol	Joback Method
hvap	81.49	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.087		Crippen Method
mcvol	160.110	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	869.17	K	Joback Method
tc	1141.62	K	Joback Method

Sources

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=C888540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
ri_{npol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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