

Ethanone, 1-(4-methoxyphenyl)-,(2,4-dinitrophenyl)hydrazone

Other names:	Acetophenone, 4'-methoxy-, (2,4-dinitrophenyl)hydrazone
Inchi:	InChI=1S/C15H14N4O5/c1-10(11-3-6-13(24-2)7-4-11)16-17-14-8-5-12(18(20)21)9-15(14)
InchiKey:	LGQWOKSOBNUYCG-UHFFFAOYSA-N
Formula:	C15H14N4O5
SMILES:	COc1ccc(C(C)=NNc2ccc([N+](=O)[O-])cc2[N+](=O)[O-])cc1
Mol. weight [g/mol]:	330.30
CAS:	854-04-6

Physical Properties

Property code	Value	Unit	Source
hf	57.88	kJ/mol	Joback Method
hvap	100.94	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.348		Crippen Method
mcvol	231.060	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
tb	1063.73	K	Joback Method
tc	1341.51	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=C854046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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