2,4-dinitrophenylhydrazone 3-methyl-3-buten-2-one

Inchi: InChI=1S/C11H12N4O4/c1-7(2)8(3)12-13-10-5-4-9(14(16)17)6-11(10)15(18)19/h4-6,13H

InchiKey: YWMNYZMUZVYIDX-UHFFFAOYSA-N

Formula: C11H12N4O4

SMILES: C=C(C)C(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]

Mol. weight [g/mol]: 264.24

Physical Properties

Property code	Value	Unit	Source
hf	163.24	kJ/mol	Joback Method
hvap	86.10	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	2.867		Crippen Method
mcvol	188.290	ml/mol	McGowan Method
pc	2527.73	kPa	Joback Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook
tb	914.69	K	Joback Method
tc	1183.56	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=R139758&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature