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

Inchi: InChI=1S/C10H12N4O4/c1-3-7(2)11-12-9-5-4-8(13(15)16)6-10(9)14(17)18/h4-6,12H,3H2
InchiKey: WPWSANGSIWAACK-UHFFFAOYSA-N
Formula: C10H12N4O4
SMILES: CCC(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]: 252.23
CAS: 958-60-1

Physical Properties

Property code	Value	Unit	Source
hf	68.24	kJ/mol	Joback Method
hvap	84.47	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.701		Crippen Method
mcvol	178.500	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	2356.00		NIST Webbook
rinpol	2325.80		NIST Webbook
rinpol	2325.80		NIST Webbook
tb	895.25	K	Joback Method
tc	1161.01	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=C958601&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