

2-Butanone,3-oxo-(2,4-dinitrophenyl)hydrazone

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|----------------------|--|
| Inchi: | InChI=1S/C10H10N4O5/c1-6(7(2)15)11-12-9-4-3-8(13(16)17)5-10(9)14(18)19/h3-5,12H, |
| InchiKey: | CMMZDRNKABQCMK-UHFFFAOYSA-N |
| Formula: | C10H10N4O5 |
| SMILES: | CC(=O)C(C)=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-] |
| Mol. weight [g/mol]: | 266.21 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| hf | -44.34 | kJ/mol | Joback Method |
| hvap | 91.21 | kJ/mol | Joback Method |
| log10ws | -3.47 | | Crippen Method |
| logp | 1.880 | | Crippen Method |
| mcvol | 180.070 | ml/mol | McGowan Method |
| pc | 2838.39 | kPa | Joback Method |
| rinpol | 2411.00 | | NIST Webbook |
| tb | 949.12 | K | Joback Method |
| tc | 1218.54 | 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=U143494&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

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|----------------|-------------------------------------|
| 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 |

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