

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

Inchi: InChI=1S/C10H12N4O5/c1-6(7(2)15)11-12-9-4-3-8(13(16)17)5-10(9)14(18)19/h3-5,7,12,
InchiKey: CWIVDHFDRDDERB-UHFFFAOYSA-N
Formula: C10H12N4O5
SMILES: CC(=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-])C(C)O
Mol. weight [g/mol]: 268.23
CAS: 35015-94-2

Physical Properties

Property code	Value	Unit	Source
hf	-89.27	kJ/mol	Joback Method
hvap	100.76	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	1.672		Crippen Method
mcvol	184.370	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
tb	986.99	K	Joback Method
tc	1239.03	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=C35015942&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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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