BENZALDEHYDE, 2,4-DINITROPHENYL HYDRAZONE

Other names: Benzaldehyde, 1-(2,4-dinitrophenyl)hydrazone
Inchi: InChI=1S/C13H10N4O4/c18-16(19)11-6-7-12(13(8-11)17(20)21)15-14-9-10-4-2-1-3-5-10
InchiKey: DZPRPFUXOZTWAJ-UHFFFAOYSA-N
Formula: C13H10N4O4
SMILES: O=[N+]([O-])c1ccc(NN=Cc2ccccc2)c([N+](=O)[O-])c1
Mol. weight [g/mol]: 286.25

Physical Properties

Property code	Value	Unit	Source
hf	333.57	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
log10ws	-4.05		Cheméo Relay (1.0)
logp	2.949		Crippen Method
mcvol	197.010	ml/mol	McGowan Method
tb	652.25	K	Cheméo Relay (1.0)
tf	429.80	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1157842&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf: Enthalpy of formation at standard conditions
ie: Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point