

Butanal, (2,4-dinitrophenyl)hydrazone

Other names:	Butyraldehyde, (2,4-dinitrophenyl)hydrazone
Inchi:	InChI=1S/C10H12N4O4/c1-2-3-6-11-12-9-5-4-8(13(15)16)7-10(9)14(17)18/h4-7,12H,2-3
InchiKey:	IKGRHEWIFBFXPP-UHFFFAOYSA-N
Formula:	C10H12N4O4
SMILES:	CCCC=NNc1ccc([N+](=O)[O-])cc1[N+](=O)[O-]
Mol. weight [g/mol]:	252.23
CAS:	1527-98-6

Physical Properties

Property code	Value	Unit	Source
hf	78.03	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.701		Crippen Method
mcvol	178.500	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	2378.00		NIST Webbook
tb	895.37	K	Joback Method
tc	1157.37	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1527986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Legend

hf: Enthalpy of formation at standard conditions

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature

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