

P-phthalaldehyde 2,4-dinitrophenyl hydrazone

Inchi: InChI=1S/C20H14N8O8/c29-25(30)15-5-7-17(19(9-15)27(33)34)23-21-11-13-1-2-14(4-3)
InchiKey: RXXJUOAGWBWKJN-IINORCHSSA-N
Formula: C20H14N8O8
SMILES: O=[N+]([O-])c1ccc(NN=Cc2ccc(C=NNc3ccc([N+](=O)[O-])cc3[N+](=O)[O-])cc2)c([N+](=O)[O-])
Mol. weight [g/mol]: 494.37
CAS: 117882-22-1

Physical Properties

Property code	Value	Unit	Source
hf	424.45	kJ/mol	Joback Method
hvap	156.12	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	4.211		Crippen Method
mcvol	322.380	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
tb	1623.00	K	Joback Method
tc	1988.47	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C117882221&Units=SI&Mask=3FFF>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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