

# Trichloroacetic acid 2-(p-nitrophenyl)-hydrazide

Inchi:	InChI=1S/C8H6Cl3N3O3/c9-8(10,11)7(15)13-12-5-1-3-6(4-2-5)14(16)17/h1-4,12H,(H,13,
InchiKey:	FNDDFBZHXSUDBM-UHFFFAOYSA-N
Formula:	C8H6Cl3N3O3
SMILES:	O=C(NNc1ccc([N+](=O)[O-])cc1)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	298.51
CAS:	116436-39-6

## Physical Properties

Property code	Value	Unit	Source
gf	171.72	kJ/mol	Joback Method
hf	-55.76	kJ/mol	Joback Method
hfus	38.46	kJ/mol	Joback Method
hvap	84.41	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	2.408		Crippen Method
mcvol	175.490	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
tb	829.21	K	Joback Method
tc	1093.73	K	Joback Method
tf	609.90	K	Joback Method
vc	0.669	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.41	J/molxK	829.21	Joback Method
cpg	429.48	J/molxK	873.30	Joback Method
cpg	435.76	J/molxK	917.38	Joback Method
cpg	441.36	J/molxK	961.47	Joback Method
cpg	446.41	J/molxK	1005.56	Joback Method
cpg	451.00	J/molxK	1049.65	Joback Method
cpg	455.26	J/molxK	1093.73	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116436396&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116436396&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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