

# Benzoic acid, 2-(2,4,6-trichlorophenyl)hydrazide

**Inchi:** InChI=1S/C13H9Cl3N2O/c14-9-6-10(15)12(11(16)7-9)17-18-13(19)8-4-2-1-3-5-8/h1-7,17  
**InchiKey:** FWASGTVTBTYRAD-UHFFFAOYSA-N  
**Formula:** C13H9Cl3N2O  
**SMILES:** O=C(NNc1c(Cl)cc(Cl)cc1Cl)c1ccccc1  
**Mol. weight [g/mol]:** 315.58  
**CAS:** 33422-33-2

## Physical Properties

Property code	Value	Unit	Source
gf	268.58	kJ/mol	Joback Method
hf	74.14	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	83.84	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.404		Crippen Method
mcvol	204.760	ml/mol	McGowan Method
pc	2856.62	kPa	Joback Method
tb	831.64	K	Joback Method
tc	1085.50	K	Joback Method
tf	439.93 ± 0.20	K	NIST Webbook
vc	0.770	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.73	J/molxK	831.64	Joback Method
cpg	508.31	J/molxK	873.95	Joback Method
cpg	516.93	J/molxK	916.26	Joback Method
cpg	524.67	J/molxK	958.57	Joback Method
cpg	531.59	J/molxK	1000.88	Joback Method
cpg	537.76	J/molxK	1043.19	Joback Method
cpg	543.26	J/molxK	1085.50	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=C33422332&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C33422332&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hvap:</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>mcvol:</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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