

# 2',4',5'-Trichloroacetanilide

<b>Other names:</b>	2,4,5-Trichloroacetanilide Acetamide, N-(2,4,5-trichlorophenyl)- N-(2,4,5-trichlorophenyl)acetamide
<b>Inchi:</b>	InChI=1S/C8H6Cl3NO/c1-4(13)12-8-3-6(10)5(9)2-7(8)11/h2-3H,1H3,(H,12,13)
<b>InchiKey:</b>	VUULTUGEJURGLB-UHFFFAOYSA-N
<b>Formula:</b>	C8H6Cl3NO
<b>SMILES:</b>	CC(=O)Nc1cc(Cl)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	238.50
<b>CAS:</b>	23627-24-9

## Physical Properties

Property code	Value	Unit	Source
gf	24.68	kJ/mol	Joback Method
hf	-112.66	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	64.00	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.605		Crippen Method
mcvol	148.090	ml/mol	McGowan Method
pc	3322.01	kPa	Joback Method
tb	640.39	K	Joback Method
tc	878.08	K	Joback Method
tf	436.25	K	Joback Method
vc	0.564	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.89	J/molxK	640.39	Joback Method
cpg	306.55	J/molxK	680.00	Joback Method
cpg	314.57	J/molxK	719.62	Joback Method
cpg	321.98	J/molxK	759.23	Joback Method
cpg	328.79	J/molxK	798.85	Joback Method
cpg	335.04	J/molxK	838.46	Joback Method

## Sources

<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=C23627249&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C23627249&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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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