

# 2,2,2',4'-Tetrachloropropionanilide

<b>Inchi:</b>	InChI=1S/C9H7Cl4NO/c1-9(12,13)8(15)14-7-3-2-5(10)4-6(7)11/h2-4H,1H3,(H,14,15)
<b>InchiKey:</b>	LYLOVGGYRYQRNQ-UHFFFAOYSA-N
<b>Formula:</b>	C9H7Cl4NO
<b>SMILES:</b>	CC(Cl)(Cl)C(=O)Nc1ccc(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	286.97
<b>CAS:</b>	56511-20-7

## Physical Properties

Property code	Value	Unit	Source
gf	33.64	kJ/mol	Joback Method
hf	-146.32	kJ/mol	Joback Method
hfus	28.40	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	4.126		Crippen Method
mcvol	174.420	ml/mol	McGowan Method
pc	2973.04	kPa	Joback Method
tb	692.49	K	Joback Method
tc	941.20	K	Joback Method
tf	467.34	K	Joback Method
vc	0.657	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.85	J/molxK	692.49	Joback Method
cpg	378.83	J/molxK	733.94	Joback Method
cpg	386.95	J/molxK	775.39	Joback Method
cpg	394.31	J/molxK	816.85	Joback Method
cpg	400.96	J/molxK	858.30	Joback Method
cpg	406.99	J/molxK	899.75	Joback Method
cpg	412.49	J/molxK	941.20	Joback Method

# Sources

<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=C56511207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56511207&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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