

# N-(4-([(anilinocarbothioyl)amino]methyl)-2,3,5,6-tet

<b>Inchi:</b>	InChI=1S/C22H18Cl4N4S2/c23-17-15(11-27-21(31)29-13-7-3-1-4-8-13)18(24)20(26)16(
<b>InchiKey:</b>	YLWRZAMVTARRNK-UHFFFAOYSA-N
<b>Formula:</b>	C22H18Cl4N4S2
<b>SMILES:</b>	S=C(NCc1c(Cl)c(Cl)c(CNC(=S)Nc2cccc2)c(Cl)c1Cl)Nc1cccc1
<b>Mol. weight [g/mol]:</b>	544.35
<b>CAS:</b>	116401-11-7

## Physical Properties

Property code	Value	Unit	Source
gf	967.40	kJ/mol	Joback Method
hf	598.75	kJ/mol	Joback Method
hfus	79.30	kJ/mol	Joback Method
hvap	131.45	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	7.273		Crippen Method
mcvol	362.540	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
tb	1298.18	K	Joback Method
tc	1592.63	K	Joback Method
tf	878.42	K	Joback Method
vc	1.351	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1051.23	J/molxK	1298.18	Joback Method
cpg	1070.12	J/molxK	1347.26	Joback Method
cpg	1090.77	J/molxK	1396.33	Joback Method
cpg	1113.52	J/molxK	1445.41	Joback Method
cpg	1138.73	J/molxK	1494.48	Joback Method
cpg	1166.74	J/molxK	1543.56	Joback Method
cpg	1197.92	J/molxK	1592.63	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=C116401117&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401117&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>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>mccvol:</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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