

# 4,4'-Methylene di-carbanilide

<b>Inchi:</b>	InChI=1S/C27H24N4O2/c32-26(28-22-7-3-1-4-8-22)30-24-15-11-20(12-16-24)19-21-13-
<b>InchiKey:</b>	AFGPVXVFZRRJGM-UHFFFAOYSA-N
<b>Formula:</b>	C27H24N4O2
<b>SMILES:</b>	O=C(Nc1ccccc1)Nc1ccc(Cc2ccc(NC(=O)Nc3ccccc3)cc2)cc1
<b>Mol. weight [g/mol]:</b>	436.51
<b>CAS:</b>	13140-83-5

## Physical Properties

Property code	Value	Unit	Source
gf	706.56	kJ/mol	Joback Method
hf	311.29	kJ/mol	Joback Method
hfus	64.67	kJ/mol	Joback Method
hvap	125.36	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.565		Crippen Method
mcvol	339.310	ml/mol	McGowan Method
pc	1829.41	kPa	Joback Method
tb	1242.26	K	Joback Method
tc	1523.32	K	Joback Method
tf	835.27	K	Joback Method
vc	1.268	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.02	J/molxK	1242.26	Joback Method
cpg	1133.74	J/molxK	1289.10	Joback Method
cpg	1143.03	J/molxK	1335.95	Joback Method
cpg	1152.12	J/molxK	1382.79	Joback Method
cpg	1161.25	J/molxK	1429.63	Joback Method
cpg	1170.67	J/molxK	1476.48	Joback Method
cpg	1180.60	J/molxK	1523.32	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=C13140835&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13140835&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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