

# Alpha<sup>2</sup>,alpha<sup>6</sup>-bis-(dimethylamino)-2,6-xylenol

<b>Other names:</b>	«alpha», «alpha»'-bis(dimethylamino)-2,6-xylenol Alpha
<b>Inchi:</b>	InChI=1S/C12H20N2O/c1-13(2)8-10-6-5-7-11(12(10)15)9-14(3)4/h5-7,15H,8-9H2,1-4H3
<b>InchiKey:</b>	VUENIEFVRKDJAS-UHFFFAOYSA-N
<b>Formula:</b>	C12H20N2O
<b>SMILES:</b>	CN(C)Cc1cccc(CN(C)C)c1O
<b>Mol. weight [g/mol]:</b>	208.30
<b>CAS:</b>	15827-34-6

## Physical Properties

Property code	Value	Unit	Source
gf	219.88	kJ/mol	Joback Method
hf	-108.20	kJ/mol	Joback Method
hfus	32.31	kJ/mol	Joback Method
hvap	62.34	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.515		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
tb	611.12	K	Joback Method
tc	817.40	K	Joback Method
tf	440.60	K	Joback Method
vc	0.602	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.70	J/molxK	611.12	Joback Method
cpg	494.53	J/molxK	645.50	Joback Method
cpg	509.37	J/molxK	679.88	Joback Method
cpg	523.31	J/molxK	714.26	Joback Method
cpg	536.43	J/molxK	748.64	Joback Method
cpg	548.82	J/molxK	783.02	Joback Method
cpg	560.55	J/molxK	817.40	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=C15827346&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15827346&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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