

# 2,5-Piperazinedione, 3,6-bis(2-methylpropyl)-, trans-

<b>Inchi:</b>	InChI=1S/C12H22N2O2/c1-7(2)5-9-11(15)14-10(6-8(3)4)12(16)13-9/h7-10H,5-6H2,1-4H
<b>InchiKey:</b>	XWYXUMDVQIOAPR-AOOOYVTPSA-N
<b>Formula:</b>	C12H22N2O2
<b>SMILES:</b>	CC(C)CC1NC(=O)C(CC(C)C)NC1=O
<b>Mol. weight [g/mol]:</b>	226.32
<b>CAS:</b>	16679-66-6

## Physical Properties

Property code	Value	Unit	Source
gf	-7.74	kJ/mol	Joback Method
hf	-467.37	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	63.66	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.062		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
tb	720.70	K	Joback Method
tc	954.38	K	Joback Method
tf	544.64	K	Joback Method
vc	0.716	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.34	J/molxK	720.70	Joback Method
cpg	601.42	J/molxK	759.65	Joback Method
cpg	620.10	J/molxK	798.59	Joback Method
cpg	637.32	J/molxK	837.54	Joback Method
cpg	653.00	J/molxK	876.48	Joback Method
cpg	667.10	J/molxK	915.43	Joback Method
cpg	679.55	J/molxK	954.38	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=C16679666&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16679666&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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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