

# Octane, 3,6-dimethyl-3,6-diphenyl

<b>Other names:</b>	Benzene, 1,1'-(1,4-diethyl-1,4-dimethyl-1,4-butanediyl)bis-
<b>Inchi:</b>	InChI=1S/C22H30/c1-5-21(3,19-13-9-7-10-14-19)17-18-22(4,6-2)20-15-11-8-12-16-20/h7
<b>InchiKey:</b>	KJSHBAGFGAQUBT-UHFFFAOYSA-N
<b>Formula:</b>	C22H30
<b>SMILES:</b>	CCC(C)(CCC(C)(CC)c1ccccc1)c1ccccc1
<b>Mol. weight [g/mol]:</b>	294.47
<b>CAS:</b>	21411-35-8

## Physical Properties

Property code	Value	Unit	Source
gf	364.86	kJ/mol	Joback Method
hf	-41.85	kJ/mol	Joback Method
hfus	25.99	kJ/mol	Joback Method
hvap	66.53	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	6.502		Crippen Method
mcvol	273.320	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
tb	749.66	K	Joback Method
tc	979.30	K	Joback Method
tf	395.38	K	Joback Method
vc	1.030	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.42	J/molxK	749.66	Joback Method
cpg	897.70	J/molxK	941.03	Joback Method
cpg	881.93	J/molxK	902.76	Joback Method
cpg	865.06	J/molxK	864.48	Joback Method
cpg	846.96	J/molxK	826.21	Joback Method
cpg	827.46	J/molxK	787.93	Joback Method
cpg	912.53	J/molxK	979.30	Joback Method
dvisc	0.0000521	Paxs	749.66	Joback Method

dvisc	0.0000728	Paxs	690.61	Joback Method
dvisc	0.0001082	Paxs	631.57	Joback Method
dvisc	0.0001746	Paxs	572.52	Joback Method
dvisc	0.0003144	Paxs	513.47	Joback Method
dvisc	0.0006599	Paxs	454.43	Joback Method
dvisc	0.0017285	Paxs	395.38	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=C21411358&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21411358&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>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</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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