

# 1,3-Dioxane, 4-phenyl-

<b>Other names:</b>	m-Dioxane, 4-phenyl- 4-Phenyl-m-dioxane 4-Phenyl-1,3-dioxane
<b>Inchi:</b>	InChI=1S/C10H12O2/c1-2-4-9(5-3-1)10-6-7-11-8-12-10/h1-5,10H,6-8H2
<b>InchiKey:</b>	RCJRILMVFLGCJY-UHFFFAOYSA-N
<b>Formula:</b>	C10H12O2
<b>SMILES:</b>	c1ccc(C2CCOCO2)cc1
<b>Mol. weight [g/mol]:</b>	164.20
<b>CAS:</b>	772-00-9

## Physical Properties

Property code	Value	Unit	Source
gf	-2.06	kJ/mol	Joback Method
hf	-222.88	kJ/mol	Joback Method
hfus	23.49	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.122		Crippen Method
mcvol	128.880	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	523.70	K	NIST Webbook
tc	773.22	K	Joback Method
tf	289.40	K	Joback Method
vc	0.463	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.25	J/molxK	528.33	Joback Method
cpg	320.24	J/molxK	569.14	Joback Method
cpg	336.94	J/molxK	609.96	Joback Method
cpg	352.38	J/molxK	650.77	Joback Method
cpg	366.63	J/molxK	691.59	Joback Method
cpg	379.73	J/molxK	732.40	Joback Method

cpg	391.73	J/mol×K	773.22	Joback Method
dvisc	0.0049478	Paxs	289.40	Joback Method
dvisc	0.0022707	Paxs	329.22	Joback Method
dvisc	0.0012328	Paxs	369.04	Joback Method
dvisc	0.0007539	Paxs	408.86	Joback Method
dvisc	0.0005031	Paxs	448.69	Joback Method
dvisc	0.0003586	Paxs	488.51	Joback Method
dvisc	0.0002690	Paxs	528.33	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=C772009&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C772009&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>dvisc:</b>	Dynamic viscosity
<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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