

# 1,3-Benzenediol, 4-propyl-

<b>Other names:</b>	4-n-Propylresorcinol 4-propylresorcinol
<b>Inchi:</b>	InChI=1S/C9H12O2/c1-2-3-7-4-5-8(10)6-9(7)11/h4-6,10-11H,2-3H2,1H3
<b>InchiKey:</b>	DJDHQJFHXLBJNF-UHFFFAOYSA-N
<b>Formula:</b>	C9H12O2
<b>SMILES:</b>	CCc1ccc(O)cc1O
<b>Mol. weight [g/mol]:</b>	152.19
<b>CAS:</b>	18979-60-7

## Physical Properties

Property code	Value	Unit	Source
gf	-171.93	kJ/mol	Joback Method
hf	-347.18	kJ/mol	Joback Method
hfus	24.67	kJ/mol	Joback Method
hvap	63.93	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	2.050		Crippen Method
mvol	125.650	ml/mol	McGowan Method
pc	4736.62	kPa	Joback Method
tb	593.24	K	Joback Method
tc	826.79	K	Joback Method
tf	441.05	K	Joback Method
vc	0.363	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.64	J/molxK	593.24	Joback Method
cpg	325.87	J/molxK	632.17	Joback Method
cpg	336.27	J/molxK	671.09	Joback Method
cpg	345.97	J/molxK	710.02	Joback Method
cpg	355.11	J/molxK	748.94	Joback Method
cpg	363.83	J/molxK	787.87	Joback Method
cpg	372.27	J/molxK	826.79	Joback Method

dvisc	0.0002757	Paxs	441.05	Joback Method
dvisc	0.0001281	Paxs	466.42	Joback Method
dvisc	0.0000644	Paxs	491.78	Joback Method
dvisc	0.0000346	Paxs	517.14	Joback Method
dvisc	0.0000197	Paxs	542.51	Joback Method
dvisc	0.0000118	Paxs	567.88	Joback Method
dvisc	0.0000074	Paxs	593.24	Joback Method

## Sources

<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>
<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=C18979607&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18979607&amp;Units=SI</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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