

# 1,2-Naphthalenediol, diacetate

<b>Inchi:</b>	InChI=1S/C14H12O4/c1-9(15)17-13-8-7-11-5-3-4-6-12(11)14(13)18-10(2)16/h3-8H,1-2H
<b>InchiKey:</b>	YLAVAANBVJPQIB-UHFFFAOYSA-N
<b>Formula:</b>	C14H12O4
<b>SMILES:</b>	CC(=O)Oc1ccc2ccccc2c1OC(C)=O
<b>Mol. weight [g/mol]:</b>	244.24
<b>CAS:</b>	6336-79-4

## Physical Properties

Property code	Value	Unit	Source
gf	-201.04	kJ/mol	Joback Method
hf	-417.23	kJ/mol	Joback Method
hfus	27.87	kJ/mol	Joback Method
hvap	70.31	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.690		Crippen Method
mcvol	179.780	ml/mol	McGowan Method
pc	2701.41	kPa	Joback Method
tb	727.92	K	Joback Method
tc	957.77	K	Joback Method
tf	476.02	K	Joback Method
vc	0.681	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.72	J/molxK	727.92	Joback Method
cpg	484.21	J/molxK	766.23	Joback Method
cpg	495.76	J/molxK	804.54	Joback Method
cpg	506.41	J/molxK	842.84	Joback Method
cpg	516.19	J/molxK	881.15	Joback Method
cpg	525.12	J/molxK	919.46	Joback Method
cpg	533.23	J/molxK	957.77	Joback Method
dvisc	0.0009310	Paxs	476.02	Joback Method
dvisc	0.0006624	Paxs	518.00	Joback Method

dvisc	0.0004960	Paxs	559.99	Joback Method
dvisc	0.0003867	Paxs	601.97	Joback Method
dvisc	0.0003115	Paxs	643.95	Joback Method
dvisc	0.0002576	Paxs	685.94	Joback Method
dvisc	0.0002177	Paxs	727.92	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=C6336794&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6336794&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>mccvol:</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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