

# gibbilimbol D

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H20O/c1-2-3-4-5-6-7-8-13-9-11-14(15)12-10-13/h5-6,9-12,15H,2-4,7-8H2,UTXMWVVQOZAGKZ-AATRIKPKSA-NC14H20OCCCCC=CCCc1ccc(O)cc1204.31

## Physical Properties

Property code	Value	Unit	Source
gf	105.01	kJ/mol	Joback Method
hf	-155.85	kJ/mol	Joback Method
hfus	32.04	kJ/mol	Joback Method
hvap	62.01	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.071		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1789.00		NIST Webbook
tb	631.18	K	Joback Method
tc	844.05	K	Joback Method
tf	380.60	K	Joback Method
vc	0.657	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.44	J/molxK	631.18	Joback Method
cpg	554.92	J/molxK	808.58	Joback Method
cpg	542.38	J/molxK	773.10	Joback Method
cpg	529.16	J/molxK	737.62	Joback Method
cpg	515.16	J/molxK	702.14	Joback Method
cpg	500.29	J/molxK	666.66	Joback Method
cpg	566.87	J/molxK	844.05	Joback Method
dvisc	0.0000204	Paxs	631.18	Joback Method
dvisc	0.0000325	Paxs	589.42	Joback Method

dvisc	0.0000555	Paxs	547.65	Joback Method
dvisc	0.0001038	Paxs	505.89	Joback Method
dvisc	0.0002173	Paxs	464.13	Joback Method
dvisc	0.0005261	Paxs	422.36	Joback Method
dvisc	0.0015468	Paxs	380.60	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=R519005&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R519005&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>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>rinpol:</b>	Non-polar retention indices
<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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