

# D-Homoestra-1,3,5(10),6,8-pentaen-17a-one,3-met

<b>Inchi:</b>	InChI=1S/C20H22O2/c1-20-10-9-17-16-7-5-15(22-2)11-13(16)3-6-18(17)19(20)8-4-14(2
<b>InchiKey:</b>	CDRSYMMICFCUFM-XJDOXCRVSA-N
<b>Formula:</b>	C20H22O2
<b>SMILES:</b>	COc1ccc2c3c(ccc2c1)C1CCC(=O)CC1(C)CC3
<b>Mol. weight [g/mol]:</b>	294.39
<b>CAS:</b>	1232-91-3

## Physical Properties

Property code	Value	Unit	Source
gf	171.91	kJ/mol	Joback Method
hf	-184.34	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	71.69	kJ/mol	Joback Method
ie	7.82 ± 0.07	eV	NIST Webbook
log10ws	-5.89		Crippen Method
logp	4.638		Crippen Method
mcvol	235.160	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
tb	830.10	K	Joback Method
tc	1086.78	K	Joback Method
tf	555.03	K	Joback Method
vc	0.890	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.35	J/mol×K	830.10	Joback Method
cpg	762.04	J/mol×K	872.88	Joback Method
cpg	782.09	J/mol×K	915.66	Joback Method
cpg	801.75	J/mol×K	958.44	Joback Method
cpg	821.27	J/mol×K	1001.22	Joback Method
cpg	840.89	J/mol×K	1044.00	Joback Method
cpg	860.87	J/mol×K	1086.78	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=C1232913&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1232913&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>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<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>ie:</b>	Ionization energy
<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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