

# Anhydroretinol

<b>Inchi:</b>	InChI=1S/C20H28/c1-7-16(2)10-8-11-17(3)13-14-19-18(4)12-9-15-20(19,5)6/h7-8,10-14H
<b>InchiKey:</b>	FWNRILWHNGFAIN-SSHGZYQJSA-N
<b>Formula:</b>	C20H28
<b>SMILES:</b>	<chem>C=CC(C)=CC=CC(C)=CC=C1C(C)=CCCC1(C)C</chem>
<b>Mol. weight [g/mol]:</b>	268.44

## Physical Properties

Property code	Value	Unit	Source
gf	513.67	kJ/mol	Joback Method
hf	193.28	kJ/mol	Joback Method
hfus	30.96	kJ/mol	Joback Method
hvap	60.50	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.314		Crippen Method
mcvol	256.000	ml/mol	McGowan Method
pc	1445.73	kPa	Joback Method
rinsol	2233.00		NIST Webbook
tb	696.49	K	Joback Method
tc	916.76	K	Joback Method
tf	325.16	K	Joback Method
vc	0.979	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.85	J/mol×K	696.49	Joback Method
cpg	719.61	J/mol×K	733.20	Joback Method
cpg	739.42	J/mol×K	769.91	Joback Method
cpg	758.47	J/mol×K	806.62	Joback Method
cpg	776.97	J/mol×K	843.33	Joback Method
cpg	795.12	J/mol×K	880.05	Joback Method
cpg	813.12	J/mol×K	916.76	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=R55533&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R55533&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>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>hvac:</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>mccol:</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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