

# 4-Chromanol

<b>Other names:</b>	Chromanol 2H-1-Benzopyran-4-ol, 3,4-dihydro- Chroman-4-ol 4-Hydroxychroman 3,4-dihydro-2H-1-benzopyran-4-ol
<b>Inchi:</b>	InChI=1S/C9H10O2/c10-8-5-6-11-9-4-2-1-3-7(8)9/h1-4,8,10H,5-6H2
<b>InchiKey:</b>	MGSHXMOLUWTMGP-UHFFFAOYSA-N
<b>Formula:</b>	C9H10O2
<b>SMILES:</b>	OC1CCOc2ccccc21
<b>Mol. weight [g/mol]:</b>	150.17
<b>CAS:</b>	1481-93-2

## Physical Properties

Property code	Value	Unit	Source
gf	-46.61	kJ/mol	Joback Method
hf	-221.62	kJ/mol	Joback Method
hfus	20.82	kJ/mol	Joback Method
hvap	59.84	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.502		Crippen Method
mcvol	114.790	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	567.12	K	Joback Method
tc	783.55	K	Joback Method
tf	331.94	K	Joback Method
vc	0.420	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.59	J/molxK	567.12	Joback Method
cpg	291.79	J/molxK	603.19	Joback Method
cpg	303.17	J/molxK	639.26	Joback Method
cpg	313.77	J/molxK	675.34	Joback Method

cpg	323.64	J/molxK	711.41	Joback Method
cpg	332.82	J/molxK	747.48	Joback Method
cpg	341.35	J/molxK	783.55	Joback Method
dvisc	0.0058458	Paxs	331.94	Joback Method
dvisc	0.0024107	Paxs	371.14	Joback Method
dvisc	0.0011775	Paxs	410.33	Joback Method
dvisc	0.0006517	Paxs	449.53	Joback Method
dvisc	0.0003966	Paxs	488.73	Joback Method
dvisc	0.0002598	Paxs	527.92	Joback Method
dvisc	0.0001804	Paxs	567.12	Joback Method

## Sources

<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=C1481932&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1481932&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>
<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>

## 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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