

# Isochroman

<b>Other names:</b>	1H-2-Benzopyran, 3,4-dihydro- isochromane
<b>Inchi:</b>	InChI=1S/C9H10O/c1-2-4-9-7-10-6-5-8(9)3-1/h1-4H,5-7H2
<b>InchiKey:</b>	HEBMCVBCEDMUOF-UHFFFAOYSA-N
<b>Formula:</b>	C9H10O
<b>SMILES:</b>	<chem>c1ccc2c(c1)CCOC2</chem>
<b>Mol. weight [g/mol]:</b>	134.18
<b>CAS:</b>	493-05-0

## Physical Properties

Property code	Value	Unit	Source
chl	-4850.50 ± 0.80	kJ/mol	NIST Webbook
gf	97.92	kJ/mol	Joback Method
hf	-63.10 ± 1.10	kJ/mol	NIST Webbook
hfl	-120.20 ± 1.10	kJ/mol	NIST Webbook
hfus	15.66	kJ/mol	Joback Method
hsub	57.10 ± 0.10	kJ/mol	NIST Webbook
hvap	57.10	kJ/mol	NIST Webbook
hvap	57.10	kJ/mol	NIST Webbook
ie	8.90	eV	NIST Webbook
log10ws	-2.14		Crippen Method
logp	1.759		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	1184.80		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1184.80		NIST Webbook
rinpol	1151.00		NIST Webbook
ripol	1751.10		NIST Webbook
ripol	1751.10		NIST Webbook
sl	247.02	J/molxK	NIST Webbook
sl	247.04	J/molxK	NIST Webbook
tb	479.61	K	Joback Method
tc	714.33	K	Joback Method
tf	277.50	K	NIST Webbook
vc	0.403	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.77	J/molxK	714.33	Joback Method
cpg	227.70	J/molxK	479.61	Joback Method
cpg	291.71	J/molxK	675.21	Joback Method
cpg	280.82	J/molxK	636.09	Joback Method
cpg	269.05	J/molxK	596.97	Joback Method
cpg	256.31	J/molxK	557.85	Joback Method
cpg	242.55	J/molxK	518.73	Joback Method
cpl	217.81	J/molxK	298.15	NIST Webbook
cpl	217.77	J/molxK	298.15	NIST Webbook
dvisc	0.0004578	Paxs	445.57	Joback Method
dvisc	0.0005841	Paxs	411.53	Joback Method
dvisc	0.0016733	Paxs	309.40	Joback Method
dvisc	0.0003715	Paxs	479.61	Joback Method
dvisc	0.0010990	Paxs	343.44	Joback Method
dvisc	0.0007787	Paxs	377.49	Joback Method
dvisc	0.0028266	Paxs	275.36	Joback Method
hfust	16.75	kJ/mol	277.50	NIST Webbook
hfust	16.75	kJ/mol	277.50	NIST Webbook
hfust	16.75	kJ/mol	277.50	NIST Webbook
hsubt	42.60 ± 0.50	kJ/mol	415.50	NIST Webbook
hsubt	45.30 ± 0.30	kJ/mol	415.50	NIST Webbook
hsubt	48.70 ± 0.10	kJ/mol	415.50	NIST Webbook
hsubt	50.30 ± 0.10	kJ/mol	415.50	NIST Webbook
hsubt	55.60 ± 0.10	kJ/mol	415.50	NIST Webbook
hsubt	52.90 ± 0.10	kJ/mol	415.50	NIST Webbook
sfust	60.35	J/molxK	277.50	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	363.20	K	1.60	NIST Webbook

# Sources

<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>
<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=C493050&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C493050&amp;Units=SI</a>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase 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>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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