

# Lyratol

<b>Inchi:</b>	InChI=1S/C10H16O/c1-5-10(8(2)3)6-9(4)7-11/h5-6,10-11H,1-2,7H2,3-4H3/b9-6+
<b>InchiKey:</b>	NHJXCMQPMLBAMK-RMKNXTFCSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	<chem>C=CC(C=C(C)CO)C(=C)C</chem>
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	19889-92-0

## Physical Properties

Property code	Value	Unit	Source
gf	132.86	kJ/mol	Joback Method
hf	-58.74	kJ/mol	Joback Method
hfus	17.24	kJ/mol	Joback Method
hvap	52.92	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.303		Crippen Method
mvol	144.730	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1164.00		NIST Webbook
tb	517.22	K	Joback Method
tc	696.85	K	Joback Method
tf	211.76	K	Joback Method
vc	0.552	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.42	J/molxK	517.22	Joback Method
cpg	337.80	J/molxK	547.16	Joback Method
cpg	349.55	J/molxK	577.10	Joback Method
cpg	360.70	J/molxK	607.04	Joback Method
cpg	371.27	J/molxK	636.98	Joback Method
cpg	381.31	J/molxK	666.91	Joback Method
cpg	390.84	J/molxK	696.85	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=C19889920&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19889920&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>rinpola:</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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