

# Licarin B

<b>Inchi:</b>	InChI=1S/C20H20O4/c1-4-5-13-8-15-12(2)19(24-20(15)18(9-13)21-3)14-6-7-16-17(10-14)
<b>InchiKey:</b>	DMMQXURQRMNSBM-SNAWJCMRSA-N
<b>Formula:</b>	C20H20O4
<b>SMILES:</b>	CC=Cc1cc(OC)c2c(c1)C(C)C(c1ccc3c(c1)OCO3)O2
<b>Mol. weight [g/mol]:</b>	324.37
<b>CAS:</b>	51020-87-2

## Physical Properties

Property code	Value	Unit	Source
gf	132.55	kJ/mol	Joback Method
hf	-305.82	kJ/mol	Joback Method
hfus	55.29	kJ/mol	Joback Method
hvap	83.70	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.694		Crippen Method
mvol	242.600	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook
tb	856.17	K	Joback Method
tc	1098.11	K	Joback Method
tf	563.34	K	Joback Method
vc	0.914	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.49	J/molxK	856.17	Joback Method
cpg	768.37	J/molxK	896.49	Joback Method
cpg	783.24	J/molxK	936.82	Joback Method
cpg	797.25	J/molxK	977.14	Joback Method
cpg	810.51	J/molxK	1017.47	Joback Method
cpg	823.15	J/molxK	1057.79	Joback Method
cpg	835.29	J/molxK	1098.11	Joback Method

dvisc	0.0013347	Paxs	563.34	Joback Method
dvisc	0.0010417	Paxs	612.14	Joback Method
dvisc	0.0008433	Paxs	660.95	Joback Method
dvisc	0.0007028	Paxs	709.76	Joback Method
dvisc	0.0005996	Paxs	758.56	Joback Method
dvisc	0.0005215	Paxs	807.37	Joback Method
dvisc	0.0004609	Paxs	856.17	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C51020872&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51020872&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mvol:</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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