

# Selina-1,3,7(11)-trien-8-one

<b>Inchi:</b>	InChI=1S/C15H20O/c1-10(2)12-8-13-11(3)6-5-7-15(13,4)9-14(12)16/h5-7,13H,8-9H2,1-4
<b>InchiKey:</b>	DVGWOFUZNUYQPS-WUJWULDRSA-N
<b>Formula:</b>	C15H20O
<b>SMILES:</b>	CC1=CC=CC2(C)CC(=O)C(=C(C)C)CC12
<b>Mol. weight [g/mol]:</b>	216.32
<b>CAS:</b>	179914-19-3

## Physical Properties

Property code	Value	Unit	Source
gf	107.64	kJ/mol	Joback Method
hf	-184.10	kJ/mol	Joback Method
hfus	16.76	kJ/mol	Joback Method
hvap	54.71	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.824		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1635.00		NIST Webbook
rinpol	1635.00		NIST Webbook
tb	651.04	K	Joback Method
tc	893.12	K	Joback Method
tf	383.17	K	Joback Method
vc	0.719	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.71	J/molxK	651.04	Joback Method
cpg	536.95	J/molxK	691.39	Joback Method
cpg	556.06	J/molxK	731.73	Joback Method
cpg	574.19	J/molxK	772.08	Joback Method
cpg	591.53	J/molxK	812.42	Joback Method
cpg	608.22	J/molxK	852.77	Joback Method
cpg	624.44	J/molxK	893.12	Joback Method

# Sources

<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=C179914193&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C179914193&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvp:</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>rinp:</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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