

# Shinflavanone

<b>Inchi:</b>	InChI=1S/C25H26O4/c1-15(2)5-6-16-13-17(7-9-20(16)26)23-14-21(27)18-8-10-22-19(24)
<b>InchiKey:</b>	NEIURIYDQMKXIG-UHFFFAOYSA-N
<b>Formula:</b>	C25H26O4
<b>SMILES:</b>	<chem>CC(C)=CCc1cc(C2CC(=O)c3ccc4c(c3O2)C=CC(C)(C)O4)ccc1O</chem>
<b>Mol. weight [g/mol]:</b>	390.47
<b>CAS:</b>	157414-03-4

## Physical Properties

Property code	Value	Unit	Source
gf	89.91	kJ/mol	Joback Method
hf	-397.43	kJ/mol	Joback Method
hfus	54.17	kJ/mol	Joback Method
hvap	104.07	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	5.792		Crippen Method
mvol	304.450	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	3328.90		NIST Webbook
rinpol	3328.90		NIST Webbook
tb	1072.48	K	Joback Method
tc	1339.34	K	Joback Method
tf	741.97	K	Joback Method
vc	1.097	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1069.95	J/molxK	1072.48	Joback Method
cpg	1096.62	J/molxK	1116.96	Joback Method
cpg	1124.80	J/molxK	1161.43	Joback Method
cpg	1154.87	J/molxK	1205.91	Joback Method
cpg	1187.20	J/molxK	1250.39	Joback Method
cpg	1222.20	J/molxK	1294.86	Joback Method
cpg	1260.24	J/molxK	1339.34	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C157414034&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C157414034&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>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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