

# Estrone-3-o-iodobenzoate

<b>Inchi:</b>	InChI=1S/C25H25IO3/c1-25-13-12-18-17-9-7-16(29-24(28)20-4-2-3-5-22(20)26)14-15(17
<b>InchiKey:</b>	MGUISTZCIADYNH-UHFFFAOYSA-N
<b>Formula:</b>	C25H25IO3
<b>SMILES:</b>	CC12CCC3c4ccc(OC(=O)c5ccccc5l)cc4CCC3C1CCC2=O
<b>Mol. weight [g/mol]:</b>	500.37
<b>CAS:</b>	91999-14-3

## Physical Properties

Property code	Value	Unit	Source
gf	202.01	kJ/mol	Joback Method
hf	-225.33	kJ/mol	Joback Method
hfus	39.10	kJ/mol	Joback Method
hvap	99.18	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	5.936		Crippen Method
mvol	317.840	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
tb	1101.28	K	Joback Method
tc	1385.79	K	Joback Method
tf	726.79	K	Joback Method
vc	1.190	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.45	J/molxK	1101.28	Joback Method
cpg	1114.01	J/molxK	1148.70	Joback Method
cpg	1140.61	J/molxK	1196.12	Joback Method
cpg	1168.67	J/molxK	1243.54	Joback Method
cpg	1198.58	J/molxK	1290.95	Joback Method
cpg	1230.76	J/molxK	1338.37	Joback Method
cpg	1265.61	J/molxK	1385.79	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=C91999143&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C91999143&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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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