

# Zotepine-M (HO-) HY2AC

<b>Inchi:</b>	InChI=1S/C18H13ClO4S/c1-10(20)22-14-4-6-17-12(7-14)8-16(23-11(2)21)15-9-13(19)3-
<b>InchiKey:</b>	JYXXABFVOOESDD-UHFFFAOYSA-N
<b>Formula:</b>	C18H13ClO4S
<b>SMILES:</b>	CC(=O)OC1=Cc2cc(OC(C)=O)ccc2Sc2ccc(Cl)cc21
<b>Mol. weight [g/mol]:</b>	360.81

## Physical Properties

Property code	Value	Unit	Source
gf	-64.14	kJ/mol	Joback Method
hf	-308.30	kJ/mol	Joback Method
hfus	40.23	kJ/mol	Joback Method
hvap	92.55	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.791		Crippen Method
mcvol	245.270	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpola	2735.00		NIST Webbook
rinpola	2735.00		NIST Webbook
rinpola	2735.00		NIST Webbook
tb	937.91	K	Joback Method
tc	1192.89	K	Joback Method
tf	688.69	K	Joback Method
vc	0.914	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.24	J/molxK	937.91	Joback Method
cpg	682.67	J/molxK	980.41	Joback Method
cpg	692.08	J/molxK	1022.90	Joback Method
cpg	700.55	J/molxK	1065.40	Joback Method
cpg	708.15	J/molxK	1107.90	Joback Method
cpg	714.95	J/molxK	1150.39	Joback Method
cpg	721.01	J/molxK	1192.89	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=R331325&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331325&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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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