

# 3-Acetoxy salicylic acid, phenyl ester

<b>Inchi:</b>	InChI=1S/C15H12O5/c1-10(16)19-13-9-5-8-12(14(13)17)15(18)20-11-6-3-2-4-7-11/h2-9,
<b>InchiKey:</b>	TVWZTHFHVCLXFL-UHFFFAOYSA-N
<b>Formula:</b>	C15H12O5
<b>SMILES:</b>	CC(=O)Oc1cccc(C(=O)Oc2ccccc2)c1O
<b>Mol. weight [g/mol]:</b>	272.25

## Physical Properties

Property code	Value	Unit	Source
gf	-331.85	kJ/mol	Joback Method
hf	-558.25	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	85.52	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.537		Crippen Method
mcvol	195.440	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	834.14	K	Joback Method
tc	1080.69	K	Joback Method
tf	580.21	K	Joback Method
vc	0.673	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.46	J/molxK	834.14	Joback Method
cpg	560.90	J/molxK	875.23	Joback Method
cpg	571.46	J/molxK	916.32	Joback Method
cpg	581.21	J/molxK	957.41	Joback Method
cpg	590.24	J/molxK	998.50	Joback Method
cpg	598.64	J/molxK	1039.59	Joback Method
cpg	606.48	J/molxK	1080.69	Joback Method
dvisc	0.0000770	Paxs	580.21	Joback Method
dvisc	0.0000429	Paxs	622.53	Joback Method
dvisc	0.0000258	Paxs	664.85	Joback Method

dvisc	0.0000165	Paxs	707.17	Joback Method
dvisc	0.0000110	Paxs	749.50	Joback Method
dvisc	0.0000077	Paxs	791.82	Joback Method
dvisc	0.0000056	Paxs	834.14	Joback Method

## Sources

<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=B6004194&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004194&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>

## 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>mcvol:</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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