

# Salicylic acid, 2-methylbutyl ether, 2-methylbutyl ester

<b>Inchi:</b>	InChI=1S/C17H26O3/c1-5-13(3)11-19-16-10-8-7-9-15(16)17(18)20-12-14(4)6-2/h7-10,13
<b>InchiKey:</b>	KVOOIWOVRWCHTQ-UHFFFAOYSA-N
<b>Formula:</b>	C17H26O3
<b>SMILES:</b>	CCC(C)COC(=O)c1ccccc1OCC(C)CC
<b>Mol. weight [g/mol]:</b>	278.39

## Physical Properties

Property code	Value	Unit	Source
gf	-148.76	kJ/mol	Joback Method
hf	-556.73	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	67.16	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.314		Crippen Method
mcvol	239.940	ml/mol	McGowan Method
pc	1614.17	kPa	Joback Method
rinsol	1929.00		NIST Webbook
tb	717.85	K	Joback Method
tc	917.15	K	Joback Method
tf	384.68	K	Joback Method
vc	0.909	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.79	J/molxK	717.85	Joback Method
cpg	702.32	J/molxK	751.07	Joback Method
cpg	718.82	J/molxK	784.28	Joback Method
cpg	734.30	J/molxK	817.50	Joback Method
cpg	748.78	J/molxK	850.72	Joback Method
cpg	762.28	J/molxK	883.94	Joback Method
cpg	774.80	J/molxK	917.15	Joback Method
dvisc	0.0013826	Paxs	384.68	Joback Method
dvisc	0.0006173	Paxs	440.21	Joback Method

dvisc	0.0003301	Paxs	495.74	Joback Method
dvisc	0.0002003	Paxs	551.26	Joback Method
dvisc	0.0001332	Paxs	606.79	Joback Method
dvisc	0.0000948	Paxs	662.32	Joback Method
dvisc	0.0000711	Paxs	717.85	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=U375429&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375429&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>rinpol:</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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