

# Sophorose, permethyl

**Inchi:** InChI=1S/C20H38O11/c1-21-9-11-14(24-4)16(26-6)18(19(28-8)29-11)31-20-17(27-7)15(23-3)  
**InchiKey:** JIBCAZMNXQQBIE-JOVUISTQSA-N  
**Formula:** C20H38O11  
**SMILES:** COCC1OC(OC2C(OC)OC(COC)C(OC)C2OC)C(OC)C(OC)C1OC  
**Mol. weight [g/mol]:** 454.51

## Physical Properties

Property code	Value	Unit	Source
gf	-1012.50	kJ/mol	Joback Method
hf	-1964.19	kJ/mol	Joback Method
hfus	66.44	kJ/mol	Joback Method
hvap	89.21	kJ/mol	Joback Method
log10ws	-0.05		Crippen Method
logp	-0.164		Crippen Method
mcvol	335.510	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
rinsol	2329.00		NIST Webbook
tb	914.42	K	Joback Method
tc	1121.61	K	Joback Method
tf	549.21	K	Joback Method
vc	1.218	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.05	J/molxK	914.42	Joback Method
cpg	1257.67	J/molxK	948.95	Joback Method
cpg	1273.53	J/molxK	983.48	Joback Method
cpg	1286.53	J/molxK	1018.01	Joback Method
cpg	1296.53	J/molxK	1052.54	Joback Method
cpg	1303.43	J/molxK	1087.07	Joback Method
cpg	1307.10	J/molxK	1121.61	Joback Method
dvisc	0.0002167	Paxs	549.21	Joback Method
dvisc	0.0001503	Paxs	610.08	Joback Method

dvisc	0.0001114	Paxs	670.95	Joback Method
dvisc	0.0000868	Paxs	731.82	Joback Method
dvisc	0.0000703	Paxs	792.68	Joback Method
dvisc	0.0000586	Paxs	853.55	Joback Method
dvisc	0.0000501	Paxs	914.42	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=R151238&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R151238&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>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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<https://www.chemeo.com/cid/13-804-4/Sophorose-permethyl.pdf>

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