

# ent-Trachyloban-3 «beta»-ol

<b>Inchi:</b>	InChI=1S/C20H32O/c1-17(2)14-5-8-20-10-13-12(19(13,4)11-20)9-15(20)18(14,3)7-6-16(
<b>InchiKey:</b>	JHYUVBXKRVZLON-SAZHDMPUSA-N
<b>Formula:</b>	C20H32O
<b>SMILES:</b>	CC1(C)C(O)CCC2(C)C3CC4C5CC3(CCC12)CC45C
<b>Mol. weight [g/mol]:</b>	288.47

## Physical Properties

Property code	Value	Unit	Source
gf	219.55	kJ/mol	Joback Method
hf	-270.92	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	70.69	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.636		Crippen Method
mcvol	244.230	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
tb	769.43	K	Joback Method
tc	992.67	K	Joback Method
tf	540.80	K	Joback Method
vc	0.940	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	847.99	J/mol×K	769.43	Joback Method
cpg	872.92	J/mol×K	806.64	Joback Method
cpg	898.55	J/mol×K	843.84	Joback Method
cpg	925.44	J/mol×K	881.05	Joback Method
cpg	954.14	J/mol×K	918.26	Joback Method
cpg	985.19	J/mol×K	955.47	Joback Method
cpg	1019.16	J/mol×K	992.67	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=R420410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R420410&amp;Units=SI</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>hvp:</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>rinp:</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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