

# trans-Verbenyl caprate

**Inchi:** InChI=1S/C20H34O2/c1-5-6-7-8-9-10-11-12-19(21)22-18-13-15(2)16-14-17(18)20(16,3)4  
**InchiKey:** XMOYMWIGBAEZME-UHFFFAOYSA-N  
**Formula:** C20H34O2  
**SMILES:** CCCCCCCCC(=O)OC1C=C(C)C2CC1C2(C)C  
**Mol. weight [g/mol]:** 306.48

## Physical Properties

Property code	Value	Unit	Source
gf	-7.58	kJ/mol	Joback Method
hf	-540.62	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	68.45	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.661		Crippen Method
mvol	274.080	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	2072.50		NIST Webbook
rinpol	2072.50		NIST Webbook
tb	746.08	K	Joback Method
tc	938.16	K	Joback Method
tf	448.38	K	Joback Method
vc	1.067	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	858.00	J/mol×K	746.08	Joback Method
cpg	878.64	J/mol×K	778.09	Joback Method
cpg	898.51	J/mol×K	810.11	Joback Method
cpg	917.71	J/mol×K	842.12	Joback Method
cpg	936.34	J/mol×K	874.14	Joback Method
cpg	954.52	J/mol×K	906.15	Joback Method
cpg	972.35	J/mol×K	938.16	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=U414147&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U414147&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>rinpolar:</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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