

# (Z)-«gamma»-Curcuml 2-methylbutanoate

<b>Inchi:</b>	InChI=1S/C20H30O3/c1-7-13(4)18(21)22-20-10-14(5)16-9-8-15(6)19(16,23-20)11-17(20)
<b>InchiKey:</b>	WUHNBNJYUGWOM-IKWVQECISA-N
<b>Formula:</b>	C20H30O3
<b>SMILES:</b>	<chem>C=C1CC2(OC(=O)C(C)CC)OC3(CC2=C(C)C)C(C)CCC13</chem>
<b>Mol. weight [g/mol]:</b>	318.45

## Physical Properties

Property code	Value	Unit	Source
gf	24.39	kJ/mol	Joback Method
hf	-471.51	kJ/mol	Joback Method
hfus	31.33	kJ/mol	Joback Method
hvap	71.89	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.774		Crippen Method
mcvol	264.790	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinsol	1902.00		NIST Webbook
tb	790.05	K	Joback Method
tc	1010.84	K	Joback Method
tf	499.31	K	Joback Method
vc	1.012	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.75	J/molxK	790.05	Joback Method
cpg	871.59	J/molxK	826.85	Joback Method
cpg	893.26	J/molxK	863.65	Joback Method
cpg	915.04	J/molxK	900.45	Joback Method
cpg	937.19	J/molxK	937.25	Joback Method
cpg	960.01	J/molxK	974.04	Joback Method
cpg	983.77	J/molxK	1010.84	Joback Method

# Sources

<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>
<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=R626638&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R626638&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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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