

# 19-Oxo-ent-kaur-16-ene

<b>Inchi:</b>	InChI=1S/C20H30O/c1-14-11-20-10-7-16-18(2,13-21)8-4-9-19(16,3)17(20)6-5-15(14)12-
<b>InchiKey:</b>	JCAVDWHQNFTFBW-GTYQWKCWSA-N
<b>Formula:</b>	C20H30O
<b>SMILES:</b>	<chem>C=C1CC23CCC4C(C)(C=O)CCCC4(C)C2CCC1C3</chem>
<b>Mol. weight [g/mol]:</b>	286.45

## Physical Properties

Property code	Value	Unit	Source
gf	233.79	kJ/mol	Joback Method
hf	-185.87	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	63.26	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	5.154		Crippen Method
mvol	246.490	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	2255.00		NIST Webbook
tb	740.24	K	Joback Method
tc	982.40	K	Joback Method
tf	491.74	K	Joback Method
vc	0.945	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.94	J/mol×K	740.24	Joback Method
cpg	822.65	J/mol×K	780.60	Joback Method
cpg	848.11	J/mol×K	820.96	Joback Method
cpg	873.84	J/mol×K	861.32	Joback Method
cpg	900.34	J/mol×K	901.68	Joback Method
cpg	928.15	J/mol×K	942.04	Joback Method
cpg	957.77	J/mol×K	982.40	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R586595&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R586595&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>rinpola:</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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