

# Ursolic aldehyde

<b>Inchi:</b>	InChI=1S/C30H48O2/c1-19-10-15-30(18-31)17-16-28(6)21(25(30)20(19)2)8-9-23-27(5)1
<b>InchiKey:</b>	VLFUANNVMXKBPF-UHFFFAOYSA-N
<b>Formula:</b>	C30H48O2
<b>SMILES:</b>	CC1CCC2(C=O)CCC3(C)C(=CCC4C5(C)CCC(O)C(C)(C)C5CCC43C)C2C1C
<b>Mol. weight [g/mol]:</b>	440.70
<b>CAS:</b>	19132-81-1

## Physical Properties

Property code	Value	Unit	Source
gf	131.05	kJ/mol	Joback Method
hf	-578.99	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	99.89	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	7.204		Crippen Method
mcvol	382.400	ml/mol	McGowan Method
pc	1068.66	kPa	Joback Method
rinpol	3615.50		NIST Webbook
rinpol	3615.50		NIST Webbook
tb	1067.55	K	Joback Method
tc	1313.80	K	Joback Method
tf	703.08	K	Joback Method
vc	1.450	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1619.57	J/molxK	1067.55	Joback Method
cpg	1680.76	J/molxK	1108.59	Joback Method
cpg	1747.99	J/molxK	1149.63	Joback Method
cpg	1822.08	J/molxK	1190.67	Joback Method
cpg	1903.83	J/molxK	1231.71	Joback Method
cpg	1994.05	J/molxK	1272.76	Joback Method
cpg	2093.54	J/molxK	1313.80	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=C19132811&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19132811&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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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