

# dinorlabd-8(20)-en-13-one

<b>Inchi:</b>	InChI=1S/C18H30O/c1-13-7-10-16-17(3,4)11-6-12-18(16,5)15(13)9-8-14(2)19/h15-16H,1
<b>InchiKey:</b>	JUSMYQGXCNCVARI-LEOMRAHMSA-N
<b>Formula:</b>	C18H30O
<b>SMILES:</b>	<chem>C=C1CCC2C(C)(C)CCCC2(C)C1CCC(C)=O</chem>
<b>Mol. weight [g/mol]:</b>	262.43

## Physical Properties

Property code	Value	Unit	Source
gf	71.54	kJ/mol	Joback Method
hf	-332.43	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.154		Crippen Method
mcvol	240.030	ml/mol	McGowan Method
pc	1625.91	kPa	Joback Method
rinpola	1961.00		NIST Webbook
rinpola	1961.00		NIST Webbook
tb	685.97	K	Joback Method
tc	904.63	K	Joback Method
tf	417.35	K	Joback Method
vc	0.909	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.37	J/mol×K	685.97	Joback Method
cpg	737.55	J/mol×K	722.41	Joback Method
cpg	759.80	J/mol×K	758.86	Joback Method
cpg	781.32	J/mol×K	795.30	Joback Method
cpg	802.36	J/mol×K	831.74	Joback Method
cpg	823.13	J/mol×K	868.18	Joback Method
cpg	843.87	J/mol×K	904.63	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R333514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R333514&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>hvpap:</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>rinppl:</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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