

# 2-Decalone,c&t

<b>Other names:</b>	2-Decalone (cis-trans) 2(1H)-Naphthalenone, octahydro- cis-2-Decalone bicyclo[4.4.0]decan-2-one
<b>Inchi:</b>	InChI=1S/C10H16O/c11-10-6-5-8-3-1-2-4-9(8)7-10/h8-9H,1-7H2/t8-,9+/m1/s1
<b>InchiKey:</b>	LGVJRKCCQQHOWAU-BDAKNGLRSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	O=C1CCC2CCCCC2C1
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	4832-17-1

## Physical Properties

Property code	Value	Unit	Source
gf	-16.17	kJ/mol	Joback Method
hf	-266.47	kJ/mol	Joback Method
hfus	9.04	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.546		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
rinpol	1275.00		NIST Webbook
tb	526.58	K	Joback Method
tc	766.02	K	Joback Method
tf	292.48	K	Joback Method
vc	0.484	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	325.13	J/mol×K	526.58	Joback Method
cpg	346.46	J/mol×K	566.49	Joback Method
cpg	366.51	J/mol×K	606.39	Joback Method
cpg	385.29	J/mol×K	646.30	Joback Method

cpg	402.83	J/mol×K	686.21	Joback Method
cpg	419.17	J/mol×K	726.11	Joback Method
cpg	434.33	J/mol×K	766.02	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	369.20	K	0.40	NIST Webbook

## Sources

<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=C4832171&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4832171&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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