

# trans-2-Ethyl-4-tert-butylcyclohexanone

<b>Inchi:</b>	InChI=1S/C12H22O/c1-5-9-8-10(12(2,3)4)6-7-11(9)13/h9-10H,5-8H2,1-4H3/t9-,10+/m1/s
<b>InchiKey:</b>	UMEJTHPXAININP-ZJUUUORDSA-N
<b>Formula:</b>	C12H22O
<b>SMILES:</b>	CCC1CC(C(C)(C)C)CCC1=O
<b>Mol. weight [g/mol]:</b>	182.30
<b>CAS:</b>	32188-06-0

## Physical Properties

Property code	Value	Unit	Source
gf	-52.85	kJ/mol	Joback Method
hf	-403.48	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	45.38	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.428		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
tb	553.43	K	Joback Method
tc	773.08	K	Joback Method
tf	298.78	K	Joback Method
vc	0.635	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.52	J/molxK	553.43	Joback Method
cpg	462.55	J/molxK	590.04	Joback Method
cpg	483.35	J/molxK	626.65	Joback Method
cpg	502.95	J/molxK	663.26	Joback Method
cpg	521.38	J/molxK	699.87	Joback Method
cpg	538.65	J/molxK	736.48	Joback Method
cpg	554.78	J/molxK	773.08	Joback Method

# Sources

<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=C32188060&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C32188060&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>

# 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>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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