

# Naphthalene, 2-(1,1-dimethylethyl)-

<b>Other names:</b>	2-(1,1-Dimethylethyl)naphthalene 2-tert-Butylnaphthalene Naphthalene, 2-tert-butyl- «beta»-tert-Butylnaphthalene Â«betaÂ»-tert-Butylnaphthalene
<b>Inchi:</b>	InChI=1S/C14H16/c1-14(2,3)13-9-8-11-6-4-5-7-12(11)10-13/h4-10H,1-3H3
<b>InchiKey:</b>	MCEORGGPAKTORV-UHFFFAOYSA-N
<b>Formula:</b>	C14H16
<b>SMILES:</b>	CC(C)(C)c1ccc2ccccc2c1
<b>Mol. weight [g/mol]:</b>	184.28
<b>CAS:</b>	2876-35-9

## Physical Properties

Property code	Value	Unit	Source
chl	-7769.50 ± 1.30	kJ/mol	NIST Webbook
gf	279.27	kJ/mol	Joback Method
hf	75.09	kJ/mol	Joback Method
hfl	-26.30 ± 1.50	kJ/mol	NIST Webbook
hfus	15.27	kJ/mol	Joback Method
hvap	50.04	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.137		Crippen Method
mcvol	164.900	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1502.00		NIST Webbook
rinpol	1475.00		NIST Webbook
tb	549.00 ± 6.00	K	NIST Webbook
tb	554.80 ± 4.00	K	NIST Webbook
tb	558.00 ± 15.00	K	NIST Webbook
tb	550.00 ± 5.00	K	NIST Webbook
tb	548.00 ± 5.00	K	NIST Webbook
tc	803.55	K	Joback Method
tf	267.00 ± 4.00	K	NIST Webbook
tf	354.00 ± 4.00	K	NIST Webbook
vc	0.623	m <sup>3</sup> /kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.23	J/molxK	567.13	Joback Method
cpg	410.99	J/molxK	606.53	Joback Method
cpg	427.37	J/molxK	645.94	Joback Method
cpg	442.47	J/molxK	685.34	Joback Method
cpg	456.40	J/molxK	724.74	Joback Method
cpg	469.28	J/molxK	764.14	Joback Method
cpg	481.23	J/molxK	803.55	Joback Method
dvisc	0.0020663	Paxs	321.60	Joback Method
dvisc	0.0011977	Paxs	362.52	Joback Method
dvisc	0.0007754	Paxs	403.44	Joback Method
dvisc	0.0005439	Paxs	444.37	Joback Method
dvisc	0.0004050	Paxs	485.29	Joback Method
dvisc	0.0003157	Paxs	526.21	Joback Method
dvisc	0.0002551	Paxs	567.13	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44790e+01
Coeff. B	-4.77092e+03
Coeff. C	-7.09660e+01
Temperature range (K), min.	407.15
Temperature range (K), max.	591.38

## Sources

The Yaws Handbook of Vapor

Pressure:  
Crippen Method:

Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

<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=C2876359&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2876359&amp;Units=SI</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase 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>pvap:</b>	Vapor 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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