

# 1,2,3-trimethyl-4-propylnaphthalene

<b>Inchi:</b>	InChI=1S/C16H20/c1-5-8-14-12(3)11(2)13(4)15-9-6-7-10-16(14)15/h6-7,9-10H,5,8H2,1-4
<b>InchiKey:</b>	ISBYEFZEJPTZHV-UHFFFAOYSA-N
<b>Formula:</b>	C16H20
<b>SMILES:</b>	CCc1c(C)c(C)c(C)c2ccccc12
<b>Mol. weight [g/mol]:</b>	212.33

## Physical Properties

Property code	Value	Unit	Source
gf	264.38	kJ/mol	Joback Method
hf	8.15	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	4.718		Crippen Method
mcvol	193.080	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinsol	284.74		NIST Webbook
tb	631.06	K	Joback Method
tc	848.12	K	Joback Method
tf	379.28	K	Joback Method
vc	0.746	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.10	J/molxK	631.06	Joback Method
cpg	506.09	J/molxK	667.24	Joback Method
cpg	522.11	J/molxK	703.41	Joback Method
cpg	537.20	J/molxK	739.59	Joback Method
cpg	551.42	J/molxK	775.77	Joback Method
cpg	564.82	J/molxK	811.94	Joback Method
cpg	577.45	J/molxK	848.12	Joback Method
dvisc	0.0010076	Paxs	379.28	Joback Method
dvisc	0.0007072	Paxs	421.24	Joback Method

dvisc	0.0005292	Paxs	463.21	Joback Method
dvisc	0.0004156	Paxs	505.17	Joback Method
dvisc	0.0003387	Paxs	547.13	Joback Method
dvisc	0.0002842	Paxs	589.10	Joback Method
dvisc	0.0002441	Paxs	631.06	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R198168&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R198168&amp;Units=SI</a>

## Legend

<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>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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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