

# 1-Tert-butyl-4-isopropylbenzene

<b>Inchi:</b>	InChI=1S/C13H20/c1-10(2)11-6-8-12(9-7-11)13(3,4)5/h6-10H,1-5H3
<b>InchiKey:</b>	QLPNXSSDHYYKBS-UHFFFAOYSA-N
<b>Formula:</b>	C13H20
<b>SMILES:</b>	CC(C)c1ccc(C(C)(C)C)cc1
<b>Mol. weight [g/mol]:</b>	176.30
<b>CAS:</b>	4132-49-4

## Physical Properties

Property code	Value	Unit	Source
gf	161.76	kJ/mol	Joback Method
hf	-100.62	kJ/mol	Joback Method
hfus	12.14	kJ/mol	Joback Method
hvap	45.79	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	4.107		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
tb	524.83	K	Joback Method
tc	739.67	K	Joback Method
tf	262.63	K	Joback Method
vc	0.638	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.59	J/molxK	524.83	Joback Method
cpg	415.56	J/molxK	560.64	Joback Method
cpg	433.35	J/molxK	596.44	Joback Method
cpg	450.02	J/molxK	632.25	Joback Method
cpg	465.63	J/molxK	668.05	Joback Method
cpg	480.24	J/molxK	703.86	Joback Method
cpg	493.91	J/molxK	739.67	Joback Method
dvisc	0.0050928	Paxs	262.63	Joback Method
dvisc	0.0019209	Paxs	306.33	Joback Method

dvisc	0.0009242	Paxs	350.03	Joback Method
dvisc	0.0005231	Paxs	393.73	Joback Method
dvisc	0.0003317	Paxs	437.43	Joback Method
dvisc	0.0002285	Paxs	481.13	Joback Method
dvisc	0.0001675	Paxs	524.83	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=C4132494&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4132494&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>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>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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