

# 1,3-Diisopropyl-5-n-Propylbenzene

<b>Inchi:</b>	InChI=1S/C13H20/c1-5-6-12-7-11(4)8-13(9-12)10(2)3/h7-10H,5-6H2,1-4H3
<b>InchiKey:</b>	HPMXLFXGBONERG-UHFFFAOYSA-N
<b>Formula:</b>	C13H20
<b>SMILES:</b>	CCc1cc(C)cc(C(C)C)c1
<b>Mol. weight [g/mol]:</b>	176.30

## Physical Properties

Property code	Value	Unit	Source
gf	149.29	kJ/mol	Joback Method
hf	-103.34	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	47.74	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.071		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2149.31	kPa	Joback Method
ripol	1512.60		NIST Webbook
tb	533.04	K	Joback Method
tc	736.09	K	Joback Method
tf	272.73	K	Joback Method
vc	0.649	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.24	J/molxK	533.04	Joback Method
cpg	472.50	J/molxK	702.25	Joback Method
cpg	458.48	J/molxK	668.41	Joback Method
cpg	443.68	J/molxK	634.57	Joback Method
cpg	428.05	J/molxK	600.72	Joback Method
cpg	411.58	J/molxK	566.88	Joback Method
cpg	485.75	J/molxK	736.09	Joback Method
dvisc	0.0001722	Paxs	533.04	Joback Method
dvisc	0.0002211	Paxs	489.65	Joback Method

dvisc	0.0002980	Paxs	446.27	Joback Method
dvisc	0.0004283	Paxs	402.88	Joback Method
dvisc	0.0006720	Paxs	359.50	Joback Method
dvisc	0.0011928	Paxs	316.12	Joback Method
dvisc	0.0025416	Paxs	272.73	Joback Method

## 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=R305589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R305589&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>
<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>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>ripol:</b>	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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