

# Tricyclobutenobenzene

<b>Other names:</b>	Tricyclobutabenzene
<b>Inchi:</b>	InChI=1S/C12H12/c1-2-8-7(1)9-3-4-11(9)12-6-5-10(8)12/h1-6H2
<b>InchiKey:</b>	MTPUNWSZJLTTLU-UHFFFAOYSA-N
<b>Formula:</b>	C12H12
<b>SMILES:</b>	C1Cc2c1c1c(c3c2CC3)CC1
<b>Mol. weight [g/mol]:</b>	156.22
<b>CAS:</b>	60323-52-6

## Physical Properties

Property code	Value	Unit	Source
gf	356.10	kJ/mol	Joback Method
hf	186.07	kJ/mol	Joback Method
hfus	16.42	kJ/mol	Joback Method
hvap	48.04	kJ/mol	Joback Method
ie	8.15 ± 0.05	eV	NIST Webbook
log10ws	-3.46		Crippen Method
logp	1.982		Crippen Method
mcvol	123.600	ml/mol	McGowan Method
pc	3460.21	kPa	Joback Method
tb	546.96	K	Joback Method
tc	777.55	K	Joback Method
tf	391.12	K	Joback Method
vc	0.497	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.35	J/molxK	546.96	Joback Method
cpg	356.79	J/molxK	739.12	Joback Method
cpg	347.01	J/molxK	700.69	Joback Method
cpg	336.54	J/molxK	662.26	Joback Method
cpg	325.22	J/molxK	623.82	Joback Method
cpg	312.88	J/molxK	585.39	Joback Method
cpg	366.07	J/molxK	777.55	Joback Method

dvisc	0.0027896	Paxs	546.96	Joback Method
dvisc	0.0027325	Paxs	520.99	Joback Method
dvisc	0.0026707	Paxs	495.01	Joback Method
dvisc	0.0026037	Paxs	469.04	Joback Method
dvisc	0.0025308	Paxs	443.07	Joback Method
dvisc	0.0024513	Paxs	417.09	Joback Method
dvisc	0.0023643	Paxs	391.12	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C60323526&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C60323526&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

## 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>ie:</b>	Ionization energy
<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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