

# Benzene, 1-bromo-2,4,5-trimethyl-

<b>Other names:</b>	5-Bromopseudocumene 2,4,5-Trimethylbromobenzene 5-Bromo-1,2,4-trimethylbenzene
<b>Inchi:</b>	InChI=1S/C9H11Br/c1-6-4-8(3)9(10)5-7(6)2/h4-5H,1-3H3
<b>InchiKey:</b>	SCZXFZRJDVZMJI-UHFFFAOYSA-N
<b>Formula:</b>	C9H11Br
<b>SMILES:</b>	Cc1cc(C)c(Br)cc1C
<b>Mol. weight [g/mol]:</b>	199.09
<b>CAS:</b>	5469-19-2

## Physical Properties

Property code	Value	Unit	Source
gf	122.74	kJ/mol	Joback Method
hf	-0.64	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.374		Crippen Method
mcvol	131.410	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
tb	507.20	K	NIST Webbook
tc	741.49	K	Joback Method
tf	314.97	K	Joback Method
vc	0.493	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.32	J/molxK	513.10	Joback Method
cpg	308.23	J/molxK	703.42	Joback Method
cpg	298.70	J/molxK	665.36	Joback Method
cpg	288.57	J/molxK	627.29	Joback Method
cpg	277.81	J/molxK	589.23	Joback Method
cpg	266.40	J/molxK	551.16	Joback Method

cpg	317.20	J/mol×K	741.49	Joback Method
dvisc	0.0002530	Paxs	513.10	Joback Method
dvisc	0.0003021	Paxs	480.08	Joback Method
dvisc	0.0003702	Paxs	447.06	Joback Method
dvisc	0.0004687	Paxs	414.04	Joback Method
dvisc	0.0006182	Paxs	381.01	Joback Method
dvisc	0.0008593	Paxs	347.99	Joback Method
dvisc	0.0012798	Paxs	314.97	Joback Method

## Sources

<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=C5469192&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5469192&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>

## 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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