

# 1-Bromo-2,5-dimethoxybenzene

<b>Other names:</b>	Benzene, 2-bromo-1,4-dimethoxy- 2-bromo-1,4-dimethoxybenzene
<b>Inchi:</b>	InChI=1S/C8H9BrO2/c1-10-6-3-4-8(11-2)7(9)5-6/h3-5H,1-2H3
<b>InchiKey:</b>	DWCGNRKFLRLWCJ-UHFFFAOYSA-N
<b>Formula:</b>	C8H9BrO2
<b>SMILES:</b>	COc1ccc(OC)c(Br)c1
<b>Mol. weight [g/mol]:</b>	217.06
<b>CAS:</b>	25245-34-5

## Physical Properties

Property code	Value	Unit	Source
gf	-86.05	kJ/mol	Joback Method
hf	-232.97	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	48.26	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.466		Crippen Method
mvol	129.060	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	530.08	K	Joback Method
tc	755.88	K	Joback Method
tf	335.64	K	Joback Method
vc	0.473	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.01	J/molxK	530.08	Joback Method
cpg	305.31	J/molxK	718.25	Joback Method
cpg	296.52	J/molxK	680.61	Joback Method
cpg	287.19	J/molxK	642.98	Joback Method
cpg	277.32	J/molxK	605.35	Joback Method
cpg	266.93	J/molxK	567.71	Joback Method
cpg	313.56	J/molxK	755.88	Joback Method

dvisc	0.0001906	Paxs	530.08	Joback Method
dvisc	0.0002298	Paxs	497.67	Joback Method
dvisc	0.0002844	Paxs	465.27	Joback Method
dvisc	0.0003634	Paxs	432.86	Joback Method
dvisc	0.0004832	Paxs	400.45	Joback Method
dvisc	0.0006754	Paxs	368.05	Joback Method
dvisc	0.0010073	Paxs	335.64	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.70	K	1.30	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C25245345&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C25245345&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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