

# 5-Bromo-2,4-dichloroanisole

<b>Inchi:</b>	InChI=1S/C7H5BrCl2O/c1-11-7-2-4(8)5(9)3-6(7)10/h2-3H,1H3
<b>InchiKey:</b>	SJIIFORJBWPNPM-UHFFFAOYSA-N
<b>Formula:</b>	C7H5BrCl2O
<b>SMILES:</b>	COc1cc(Br)c(Cl)cc1Cl
<b>Mol. weight [g/mol]:</b>	255.92

## Physical Properties

Property code	Value	Unit	Source
gf	-22.96	kJ/mol	Joback Method
hf	-123.06	kJ/mol	Joback Method
hfus	21.63	kJ/mol	Joback Method
hvap	53.05	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.764		Crippen Method
mcvol	133.580	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1567.00		NIST Webbook
tb	564.62	K	Joback Method
tc	808.13	K	Joback Method
tf	374.50	K	Joback Method
vc	0.497	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.46	J/mol×K	564.62	Joback Method
cpg	242.60	J/mol×K	605.20	Joback Method
cpg	250.24	J/mol×K	645.79	Joback Method
cpg	257.38	J/mol×K	686.37	Joback Method
cpg	264.05	J/mol×K	726.96	Joback Method
cpg	270.24	J/mol×K	767.54	Joback Method
cpg	275.96	J/mol×K	808.13	Joback Method
dvisc	0.0009926	Paxs	374.50	Joback Method

dvisc	0.0007114	Paxs	406.19	Joback Method
dvisc	0.0005351	Paxs	437.87	Joback Method
dvisc	0.0004183	Paxs	469.56	Joback Method
dvisc	0.0003373	Paxs	501.25	Joback Method
dvisc	0.0002790	Paxs	532.93	Joback Method
dvisc	0.0002358	Paxs	564.62	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=R323661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R323661&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>

## 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>rinpol:</b>	Non-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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