

# 2,6-Dibromo-4-nitrotoluene

<b>Inchi:</b>	InChI=1S/C7H5Br2NO2/c1-4-6(8)2-5(10(11)12)3-7(4)9/h2-3H,1H3
<b>InchiKey:</b>	HGDQAFSQPJIFA-UHFFFAOYSA-N
<b>Formula:</b>	C7H5Br2NO2
<b>SMILES:</b>	Cc1c(Br)cc([N+](=O)[O-])cc1Br
<b>Mol. weight [g/mol]:</b>	294.93
<b>CAS:</b>	110127-07-6

## Physical Properties

Property code	Value	Unit	Source
gf	155.77	kJ/mol	Joback Method
hf	56.21	kJ/mol	Joback Method
hfus	28.69	kJ/mol	Joback Method
hvap	64.90	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.428		Crippen Method
mcvol	138.150	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	685.34	K	Joback Method
tc	963.22	K	Joback Method
tf	495.84	K	Joback Method
vc	0.525	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.74	J/molxK	685.34	Joback Method
cpg	281.88	J/molxK	731.65	Joback Method
cpg	289.31	J/molxK	777.97	Joback Method
cpg	296.10	J/molxK	824.28	Joback Method
cpg	302.31	J/molxK	870.60	Joback Method
cpg	308.02	J/molxK	916.91	Joback Method
cpg	313.28	J/molxK	963.22	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C110127076&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C110127076&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>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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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