

# 1,3-Dibromo-5-fluorobenzene

<b>Inchi:</b>	InChI=1S/C6H3Br2F/c7-4-1-5(8)3-6(9)2-4/h1-3H
<b>InchiKey:</b>	ASWYHZXKFSNLN-UHFFFAOYSA-N
<b>Formula:</b>	C6H3Br2F
<b>SMILES:</b>	Fc1cc(Br)cc(Br)c1
<b>Mol. weight [g/mol]:</b>	253.89
<b>CAS:</b>	1435-51-4

## Physical Properties

Property code	Value	Unit	Source
gf	-73.38	kJ/mol	Joback Method
hf	-97.03	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	44.60	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.351		Crippen Method
mcvol	108.410	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
tb	504.91	K	Joback Method
tc	748.62	K	Joback Method
tf	329.03	K	Joback Method
vc	0.406	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.55	J/molxK	504.91	Joback Method
cpg	178.77	J/molxK	545.53	Joback Method
cpg	185.41	J/molxK	586.15	Joback Method
cpg	191.50	J/molxK	626.77	Joback Method
cpg	197.08	J/molxK	667.39	Joback Method
cpg	202.20	J/molxK	708.00	Joback Method
cpg	206.91	J/molxK	748.62	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=C1435514&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1435514&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>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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