

# 1-Bromo-3,5-difluorobenzene

<b>Other names:</b>	Benzene, 1-bromo-3,5-difluoro-
<b>Inchi:</b>	InChI=1S/C6H3BrF2/c7-4-1-5(8)3-6(9)2-4/h1-3H
<b>InchiKey:</b>	JHLKSIOJYMGSMB-UHFFFAOYSA-N
<b>Formula:</b>	C6H3BrF2
<b>SMILES:</b>	Fc1cc(F)cc(Br)c1
<b>Mol. weight [g/mol]:</b>	192.99
<b>CAS:</b>	461-96-1

## Physical Properties

Property code	Value	Unit	Source
gf	-282.51	kJ/mol	Joback Method
hf	-319.47	kJ/mol	Joback Method
hfus	16.00	kJ/mol	Joback Method
hvap	37.35	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.727		Crippen Method
mcvol	92.680	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
tb	413.20	K	NIST Webbook
tb	413.00	K	NIST Webbook
tc	651.05	K	Joback Method
tf	269.82	K	Joback Method
vc	0.361	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.73	J/molxK	438.02	Joback Method
cpg	160.24	J/molxK	473.53	Joback Method
cpg	167.26	J/molxK	509.03	Joback Method
cpg	173.84	J/molxK	544.54	Joback Method
cpg	179.98	J/molxK	580.04	Joback Method
cpg	185.71	J/molxK	615.55	Joback Method
cpg	191.05	J/molxK	651.05	Joback Method

# Sources

<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=C461961&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C461961&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>

# 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>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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