

# Cyclohexane, 1-bromo-2-fluoro-, cis-

<b>Other names:</b>	cis-1-Bromo-2-Fluorocyclohexane cis-2-Fluorocyclohexyl Bromide
<b>Inchi:</b>	InChI=1S/C6H10BrF/c7-5-3-1-2-4-6(5)8/h5-6H,1-4H2/t5-,6+/m0/s1
<b>InchiKey:</b>	AZQRVGXSORXOCR-NTSWFWBYSAN
<b>Formula:</b>	C6H10BrF
<b>SMILES:</b>	FC1CCCCC1Br
<b>Mol. weight [g/mol]:</b>	181.05
<b>CAS:</b>	51422-74-3

## Physical Properties

Property code	Value	Unit	Source
gf	-164.11	kJ/mol	Joback Method
hf	-302.97	kJ/mol	Joback Method
hfus	12.57	kJ/mol	Joback Method
hvap	34.69	kJ/mol	Joback Method
ie	10.06	eV	NIST Webbook
ie	10.04 ± 0.02	eV	NIST Webbook
log10ws	-2.74		Crippen Method
logp	2.662		Crippen Method
mcvol	103.810	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	416.99	K	Joback Method
tc	630.08	K	Joback Method
tf	220.91	K	Joback Method
vc	0.384	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.59	J/mol×K	416.99	Joback Method
cpg	199.93	J/mol×K	452.50	Joback Method
cpg	213.50	J/mol×K	488.02	Joback Method
cpg	226.33	J/mol×K	523.53	Joback Method
cpg	238.42	J/mol×K	559.05	Joback Method

cpg	249.81	J/mol×K	594.56	Joback Method
cpg	260.51	J/mol×K	630.08	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C51422743&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51422743&amp;Units=SI</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>hvac:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<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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