

# Butane, 2-bromo-3-fluoro-, (r\*,r\*)-

<b>Inchi:</b>	InChI=1S/C4H8BrF/c1-3(5)4(2)6/h3-4H,1-2H3/t3-,4-/m0/s1
<b>InchiKey:</b>	MVQSVOOVCVGPJU-IMJSIDKUSA-N
<b>Formula:</b>	C4H8BrF
<b>SMILES:</b>	CC(F)C(C)Br
<b>Mol. weight [g/mol]:</b>	155.01
<b>CAS:</b>	57302-15-5

## Physical Properties

Property code	Value	Unit	Source
gf	-202.57	kJ/mol	Joback Method
hf	-306.23	kJ/mol	Joback Method
hfus	7.43	kJ/mol	Joback Method
hvap	29.34	kJ/mol	Joback Method
ie	10.91	eV	NIST Webbook
log10ws	-2.01		Crippen Method
logp	2.128		Crippen Method
mcvol	86.490	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	355.47	K	Joback Method
tc	539.31	K	Joback Method
tf	165.23	K	Joback Method
vc	0.328	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.56	J/molxK	355.47	Joback Method
cpg	143.62	J/molxK	386.11	Joback Method
cpg	151.31	J/molxK	416.75	Joback Method
cpg	158.62	J/molxK	447.39	Joback Method
cpg	165.59	J/molxK	478.03	Joback Method
cpg	172.22	J/molxK	508.67	Joback Method
cpg	178.52	J/molxK	539.31	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=C57302155&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57302155&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>hvap:</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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