

# 2-Fluorobenzyl mercaptan

<b>Inchi:</b>	InChI=1S/C7H7FS/c8-7-4-2-1-3-6(7)5-9/h1-4,9H,5H2
<b>InchiKey:</b>	UMJTYEUXQGJEIZ-UHFFFAOYSA-N
<b>Formula:</b>	C7H7FS
<b>SMILES:</b>	Fc1ccccc1CS
<b>Mol. weight [g/mol]:</b>	142.19
<b>CAS:</b>	655-20-9

## Physical Properties

Property code	Value	Unit	Source
gf	-54.58	kJ/mol	Joback Method
hf	-120.38	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	40.03	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.256		Crippen Method
mcvol	103.850	ml/mol	McGowan Method
pc	4135.61	kPa	Joback Method
tb	453.35	K	Joback Method
tc	680.44	K	Joback Method
tf	244.64	K	Joback Method
vc	0.392	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.92	J/molxK	453.35	Joback Method
cpg	200.73	J/molxK	491.20	Joback Method
cpg	210.87	J/molxK	529.05	Joback Method
cpg	220.35	J/molxK	566.89	Joback Method
cpg	229.22	J/molxK	604.74	Joback Method
cpg	237.48	J/molxK	642.59	Joback Method
cpg	245.18	J/molxK	680.44	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=C655209&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C655209&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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