

# Phenothiazine-1-carboxylic acid, 8-trifluoromethyl-

<b>Inchi:</b>	InChI=1S/C14H8F3NO2S/c15-14(16,17)7-4-5-10-9(6-7)18-12-8(13(19)20)2-1-3-11(12)21
<b>InchiKey:</b>	WXIGSVFQTLVMQM-UHFFFAOYSA-N
<b>Formula:</b>	C14H8F3NO2S
<b>SMILES:</b>	O=C(O)c1cccc2c1Nc1cc(C(F)(F)F)ccc1S2
<b>Mol. weight [g/mol]:</b>	311.28
<b>CAS:</b>	7220-56-6

## Physical Properties

Property code	Value	Unit	Source
gf	-385.90	kJ/mol	Joback Method
hf	-584.63	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	86.26	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.612		Crippen Method
mcvol	188.820	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	837.15	K	Joback Method
tc	1067.49	K	Joback Method
tf	679.58	K	Joback Method
vc	0.721	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.40	J/molxK	837.15	Joback Method
cpg	526.18	J/molxK	875.54	Joback Method
cpg	534.44	J/molxK	913.93	Joback Method
cpg	542.28	J/molxK	952.32	Joback Method
cpg	549.82	J/molxK	990.71	Joback Method
cpg	557.16	J/molxK	1029.10	Joback Method
cpg	564.43	J/molxK	1067.49	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=C7220566&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7220566&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>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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