

# 4-(Methylthio)benzoic pentafluoropropionic anhydride

Inchi:	InChI=1S/C11H7F5O3S/c1-20-7-4-2-6(3-5-7)8(17)19-9(18)10(12,13)11(14,15)16/h2-5H,
InchiKey:	WPPUTRGFQKEJQQ-UHFFFAOYSA-N
Formula:	C11H7F5O3S
SMILES:	CSc1ccc(C(=O)OC(=O)C(F)(F)C(F)(F)F)cc1
Mol. weight [g/mol]:	314.23

## Physical Properties

Property code	Value	Unit	Source
gf	-1153.57	kJ/mol	Joback Method
hf	-1358.87	kJ/mol	Joback Method
hfus	26.99	kJ/mol	Joback Method
hvap	59.06	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.289		Crippen Method
mcvol	176.300	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
tb	671.57	K	Joback Method
tc	880.94	K	Joback Method
tf	416.95	K	Joback Method
vc	0.696	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.96	J/molxK	671.57	Joback Method
cpg	469.43	J/molxK	706.47	Joback Method
cpg	479.01	J/molxK	741.36	Joback Method
cpg	487.73	J/molxK	776.26	Joback Method
cpg	495.65	J/molxK	811.15	Joback Method
cpg	502.81	J/molxK	846.05	Joback Method
cpg	509.28	J/molxK	880.94	Joback Method

# Sources

<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=U374983&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374983&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>h vap:</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>r in pol:</b>	Non-polar retention indices
<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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