

# 3-(Methylthio)benzoic trifluoroacetic anhydride

Inchi:	InChI=1S/C10H7F3O3S/c1-17-7-4-2-3-6(5-7)8(14)16-9(15)10(11,12)13/h2-5H,1H3
InchiKey:	YMQQYCKKZMRIFR-UHFFFAOYSA-N
Formula:	C10H7F3O3S
SMILES:	CSc1cccc(C(=O)OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]:	264.22

## Physical Properties

Property code	Value	Unit	Source
gf	-775.21	kJ/mol	Joback Method
hf	-937.26	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	59.76	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.654		Crippen Method
mvol	158.670	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1422.00		NIST Webbook
rinpol	1422.00		NIST Webbook
tb	653.38	K	Joback Method
tc	873.50	K	Joback Method
tf	402.08	K	Joback Method
vc	0.615	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.71	J/mol×K	653.38	Joback Method
cpg	401.29	J/mol×K	690.07	Joback Method
cpg	411.02	J/mol×K	726.75	Joback Method
cpg	419.92	J/mol×K	763.44	Joback Method
cpg	428.03	J/mol×K	800.12	Joback Method
cpg	435.37	J/mol×K	836.81	Joback Method
cpg	441.97	J/mol×K	873.50	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=U374988&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374988&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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