

# 3-(Methylthio)benzoic heptafluorobutyric anhydride

Inchi:	InChI=1S/C12H7F7O3S/c1-23-7-5-3-2-4-6(7)8(20)22-9(21)10(13,14)11(15,16)12(17,18)
InchiKey:	IMGNOGMIQTVSJA-UHFFFAOYSA-N
Formula:	C12H7F7O3S
SMILES:	CSc1ccccc1C(=O)OC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	364.24

## Physical Properties

Property code	Value	Unit	Source
gf	-1531.93	kJ/mol	Joback Method
hf	-1780.48	kJ/mol	Joback Method
hfus	28.32	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.925		Crippen Method
mcvol	193.930	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1474.00		NIST Webbook
rinpol	1474.00		NIST Webbook
tb	689.76	K	Joback Method
tc	890.03	K	Joback Method
tf	431.82	K	Joback Method
vc	0.776	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.86	J/molxK	689.76	Joback Method
cpg	538.14	J/molxK	723.14	Joback Method
cpg	547.49	J/molxK	756.52	Joback Method
cpg	555.99	J/molxK	789.89	Joback Method
cpg	563.69	J/molxK	823.27	Joback Method
cpg	570.67	J/molxK	856.65	Joback Method
cpg	576.98	J/molxK	890.03	Joback Method

# Sources

<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=U374986&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374986&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>

# 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>hvp:</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>rinp:</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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