

# Methyl salicylate, O-heptafluorobutyryl-

<b>Inchi:</b>	InChI=1S/C12H7F7O4/c1-22-8(20)6-4-2-3-5-7(6)23-9(21)10(13,14)11(15,16)12(17,18)19
<b>InchiKey:</b>	LDVFFYMTANOVAI-UHFFFAOYSA-N
<b>Formula:</b>	C12H7F7O4
<b>SMILES:</b>	<chem>COC(=O)c1ccccc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F</chem>
<b>Mol. weight [g/mol]:</b>	348.17

## Physical Properties

Property code	Value	Unit	Source
gf	-1670.05	kJ/mol	Joback Method
hf	-1954.57	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	53.95	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.211		Crippen Method
mvol	183.450	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rmpol	1277.00		NIST Webbook
rmpol	1277.00		NIST Webbook
tb	643.40	K	Joback Method
tc	828.09	K	Joback Method
tf	419.65	K	Joback Method
vc	0.741	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.86	J/molxK	643.40	Joback Method
cpg	513.65	J/molxK	674.18	Joback Method
cpg	523.62	J/molxK	704.96	Joback Method
cpg	532.79	J/molxK	735.75	Joback Method
cpg	541.23	J/molxK	766.53	Joback Method
cpg	548.97	J/molxK	797.31	Joback Method
cpg	556.06	J/molxK	828.09	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=U374613&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374613&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>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>rinpola:</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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