

# 3-(Methylthio)benzoic acid, 3-chlorobenzyl ester

Inchi:	InChI=1S/C15H13ClO2S/c1-19-14-7-3-5-12(9-14)15(17)18-10-11-4-2-6-13(16)8-11/h2-9
InchiKey:	GHUVWJVYOSAVKS-UHFFFAOYSA-N
Formula:	C15H13ClO2S
SMILES:	CSc1cccc(C(=O)OCc2cccc(Cl)c2)c1
Mol. weight [g/mol]:	292.78

## Physical Properties

Property code	Value	Unit	Source
gf	68.25	kJ/mol	Joback Method
hf	-121.48	kJ/mol	Joback Method
hfus	33.02	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.419		Crippen Method
mcvol	210.720	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	2442.00		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	788.42	K	Joback Method
tc	1044.88	K	Joback Method
tf	473.17	K	Joback Method
vc	0.786	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.93	J/mol×K	788.42	Joback Method
cpg	553.03	J/mol×K	831.16	Joback Method
cpg	564.83	J/mol×K	873.91	Joback Method
cpg	575.37	J/mol×K	916.65	Joback Method
cpg	584.69	J/mol×K	959.39	Joback Method
cpg	592.82	J/mol×K	1002.14	Joback Method
cpg	599.81	J/mol×K	1044.88	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U375058&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375058&amp;Units=SI</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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