

# 4-(Methylthio)benzoic acid, 2-(2-chlorophenoxy)ethyl ester

**Inchi:** InChI=1S/C16H15ClO3S/c1-21-13-8-6-12(7-9-13)16(18)20-11-10-19-15-5-3-2-4-14(15)1

**InchiKey:** BSMSMZBEJKVDFL-UHFFFAOYSA-N

**Formula:** C16H15ClO3S

**SMILES:** CSc1ccc(C(=O)OCCOc2ccccc2Cl)cc1

**Mol. weight [g/mol]:** 322.81

## Physical Properties

Property code	Value	Unit	Source
gf	-28.33	kJ/mol	Joback Method
hf	-274.34	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.298		Crippen Method
mcvol	230.680	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpol	2715.00		NIST Webbook
rinpol	2715.00		NIST Webbook
tb	833.72	K	Joback Method
tc	1081.21	K	Joback Method
tf	506.67	K	Joback Method
vc	0.861	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.36	J/molxK	833.72	Joback Method
cpg	632.12	J/molxK	874.97	Joback Method
cpg	643.51	J/molxK	916.22	Joback Method
cpg	653.56	J/molxK	957.47	Joback Method
cpg	662.28	J/molxK	998.72	Joback Method
cpg	669.69	J/molxK	1039.97	Joback Method
cpg	675.81	J/molxK	1081.21	Joback Method

# Sources

<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=U375078&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375078&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>hvac:</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>rinpol:</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

Latest version available from:

<https://www.cheméo.com/cid/124-332-5/4-Methylthio-benzoic-acid-2-2-chlorophenoxy-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-29 12:44:50.780214453 +0000 UTC m=+16683939.700791768.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.