

# (Phenylthio)acetic acid, 3-tridecyl ester

<b>Inchi:</b>	InChI=1S/C21H34O2S/c1-3-5-6-7-8-9-10-12-15-19(4-2)23-21(22)18-24-20-16-13-11-14-
<b>InchiKey:</b>	ICBAPICAECJEJN-UHFFFAOYSA-N
<b>Formula:</b>	C21H34O2S
<b>SMILES:</b>	CCCCCCCCCCC(CC)OC(=O)CSc1ccccc1
<b>Mol. weight [g/mol]:</b>	350.56

## Physical Properties

Property code	Value	Unit	Source
gf	35.11	kJ/mol	Joback Method
hf	-448.45	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.631		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1246.85	kPa	Joback Method
tb	851.19	K	Joback Method
tc	1057.19	K	Joback Method
tf	444.41	K	Joback Method
vc	1.175	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.48	J/molxK	851.19	Joback Method
cpg	969.04	J/molxK	885.52	Joback Method
cpg	985.35	J/molxK	919.86	Joback Method
cpg	1000.48	J/molxK	954.19	Joback Method
cpg	1014.44	J/molxK	988.52	Joback Method
cpg	1027.30	J/molxK	1022.86	Joback Method
cpg	1039.08	J/molxK	1057.19	Joback Method

# Sources

<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.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=U299905&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299905&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>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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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