

# 2,4-Bis(prenylthio)but-2-enal

<b>Inchi:</b>	InChI=1S/C14H22OS2/c1-12(2)5-8-16-9-7-14(11-15)17-10-6-13(3)4/h5-7,11H,8-10H2,1-
<b>InchiKey:</b>	WHZPXKZANOPZGE-AUWJEWJLSA-N
<b>Formula:</b>	C14H22OS2
<b>SMILES:</b>	CC(C)=CCSCC=C(C=O)SCC=C(C)C
<b>Mol. weight [g/mol]:</b>	270.45

## Physical Properties

Property code	Value	Unit	Source
gf	248.73	kJ/mol	Joback Method
hf	-11.84	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	4.468		Crippen Method
mvol	229.490	ml/mol	McGowan Method
pc	1918.62	kPa	Joback Method
ripol	2750.00		NIST Webbook
ripol	2750.00		NIST Webbook
tb	718.06	K	Joback Method
tc	942.22	K	Joback Method
tf	301.22	K	Joback Method
vc	0.887	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.88	J/mol×K	718.06	Joback Method
cpg	611.50	J/mol×K	755.42	Joback Method
cpg	626.14	J/mol×K	792.78	Joback Method
cpg	639.87	J/mol×K	830.14	Joback Method
cpg	652.77	J/mol×K	867.50	Joback Method
cpg	664.93	J/mol×K	904.86	Joback Method
cpg	676.40	J/mol×K	942.22	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=R402056&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R402056&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>
<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>h vap:</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>ri pol:</b>	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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