

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

<b>Inchi:</b>	InChI=1S/C12H22OS2/c1-3-5-8-14-10-7-12(11-13)15-9-6-4-2/h7,11H,3-6,8-10H2,1-2H3
<b>InchiKey:</b>	KHFNBOJFSNECKE-GHXNOFRVSA-N
<b>Formula:</b>	C12H22OS2
<b>SMILES:</b>	CCCCSCC=C(C=O)SCCCC
<b>Mol. weight [g/mol]:</b>	246.43

## Physical Properties

Property code	Value	Unit	Source
gf	88.55	kJ/mol	Joback Method
hf	-185.42	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	62.70	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	4.136		Crippen Method
mvol	209.910	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
ripol	2587.00		NIST Webbook
ripol	2587.00		NIST Webbook
tb	664.22	K	Joback Method
tc	872.54	K	Joback Method
tf	316.76	K	Joback Method
vc	0.814	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.55	J/mol×K	664.22	Joback Method
cpg	551.95	J/mol×K	698.94	Joback Method
cpg	566.46	J/mol×K	733.66	Joback Method
cpg	580.11	J/mol×K	768.38	Joback Method
cpg	592.94	J/mol×K	803.10	Joback Method
cpg	604.97	J/mol×K	837.82	Joback Method
cpg	616.23	J/mol×K	872.54	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=R401979&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R401979&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>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>ripol:</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

Latest version available from:

<https://www.cheméo.com/cid/93-789-4/2-4-Bis-butylthio-but-2-enal.pdf>

Generated by Cheméo on 2024-04-19 18:50:04.675365769 +0000 UTC m=+15841853.595943082.

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