

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

<b>Inchi:</b>	InChI=1S/C8H14OS2/c1-3-10-6-5-8(7-9)11-4-2/h5,7H,3-4,6H2,1-2H3/b8-5-
<b>InchiKey:</b>	BRUDYKVOXQIHKT-YVMONPNESA-N
<b>Formula:</b>	C8H14OS2
<b>SMILES:</b>	CCSCC=C(C=O)SCC
<b>Mol. weight [g/mol]:</b>	190.33

## Physical Properties

Property code	Value	Unit	Source
gf	54.87	kJ/mol	Joback Method
hf	-102.86	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	53.79	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.575		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
ripol	1916.00		NIST Webbook
ripol	1916.00		NIST Webbook
tb	572.70	K	Joback Method
tc	795.53	K	Joback Method
tf	271.68	K	Joback Method
vc	0.590	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.91	J/mol×K	572.70	Joback Method
cpg	352.60	J/mol×K	609.84	Joback Method
cpg	364.54	J/mol×K	646.98	Joback Method
cpg	375.76	J/mol×K	684.11	Joback Method
cpg	386.27	J/mol×K	721.25	Joback Method
cpg	396.11	J/mol×K	758.39	Joback Method
cpg	405.29	J/mol×K	795.53	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.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=R401984&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R401984&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>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

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