

# Octacosane, 1,2-bis(methylthio)

**Inchi:** InChI=1S/C30H62S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25  
**InchiKey:** BUBWPNSHJBSWME-UHFFFAOYSA-N  
**Formula:** C30H62S2  
**SMILES:** CCCCCCCCCCCCCCCCCCCCCCCCCCCCC(CSC)SC  
**Mol. weight [g/mol]:** 486.94

## Physical Properties

Property code	Value	Unit	Source
gf	265.52	kJ/mol	Joback Method
hf	-584.07	kJ/mol	Joback Method
hfus	78.19	kJ/mol	Joback Method
hvap	95.62	kJ/mol	Joback Method
log10ws	-12.26		Crippen Method
logp	11.853		Crippen Method
mvol	466.260	ml/mol	McGowan Method
pc	607.86	kPa	Joback Method
rinpol	3626.00		NIST Webbook
rinpol	3626.00		NIST Webbook
tb	1022.92	K	Joback Method
tc	1265.28	K	Joback Method
tf	481.66	K	Joback Method
vc	1.817	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1635.49	J/mol×K	1022.92	Joback Method
cpg	1659.79	J/mol×K	1063.31	Joback Method
cpg	1682.11	J/mol×K	1103.71	Joback Method
cpg	1702.58	J/mol×K	1144.10	Joback Method
cpg	1721.29	J/mol×K	1184.49	Joback Method
cpg	1738.38	J/mol×K	1224.89	Joback Method
cpg	1753.94	J/mol×K	1265.28	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=R59317&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R59317&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>rinpola:</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

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