

# Hexacosane, 1,2-bis(methylthio)

**Inchi:** InChI=1S/C28H58S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25  
**InchiKey:** NSICRTSHVHWNQQ-UHFFFAOYSA-N  
**Formula:** C28H58S2  
**SMILES:** CCCCCCCCCCCCCCCCCCCCCCCCC(CSC)SC  
**Mol. weight [g/mol]:** 458.89

## Physical Properties

Property code	Value	Unit	Source
gf	248.68	kJ/mol	Joback Method
hf	-542.79	kJ/mol	Joback Method
hfus	73.01	kJ/mol	Joback Method
hvap	91.17	kJ/mol	Joback Method
log10ws	-11.42		Crippen Method
logp	11.073		Crippen Method
mcvol	438.080	ml/mol	McGowan Method
pc	669.77	kPa	Joback Method
rinpola	3425.00		NIST Webbook
tb	977.16	K	Joback Method
tc	1200.54	K	Joback Method
tf	459.12	K	Joback Method
vc	1.706	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1503.26	J/mol×K	977.16	Joback Method
cpg	1526.29	J/mol×K	1014.39	Joback Method
cpg	1547.62	J/mol×K	1051.62	Joback Method
cpg	1567.33	J/mol×K	1088.85	Joback Method
cpg	1585.51	J/mol×K	1126.08	Joback Method
cpg	1602.25	J/mol×K	1163.31	Joback Method
cpg	1617.61	J/mol×K	1200.54	Joback Method

# Sources

<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=R59139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R59139&amp;Units=SI</a>
<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>

# 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>rinpol:</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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