

# Heptacosane, 1,2-bis(methylthio)

<b>Inchi:</b>	InChI=1S/C29H60S2/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
<b>InchiKey:</b>	PBEZLURWEZPKNP-UHFFFAOYSA-N
<b>Formula:</b>	C29H60S2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCCCCCCCCC(CSC)SC
<b>Mol. weight [g/mol]:</b>	472.92

## Physical Properties

Property code	Value	Unit	Source
gf	257.10	kJ/mol	Joback Method
hf	-563.43	kJ/mol	Joback Method
hfus	75.60	kJ/mol	Joback Method
hvap	93.39	kJ/mol	Joback Method
log10ws	-11.84		Crippen Method
logp	11.463		Crippen Method
mvol	452.170	ml/mol	McGowan Method
pc	637.69	kPa	Joback Method
rinpol	3525.00		NIST Webbook
rinpol	3525.00		NIST Webbook
tb	1000.04	K	Joback Method
tc	1232.26	K	Joback Method
tf	470.39	K	Joback Method
vc	1.762	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1569.21	J/mol×K	1000.04	Joback Method
cpg	1592.84	J/mol×K	1038.74	Joback Method
cpg	1614.64	J/mol×K	1077.45	Joback Method
cpg	1634.71	J/mol×K	1116.15	Joback Method
cpg	1653.15	J/mol×K	1154.85	Joback Method
cpg	1670.05	J/mol×K	1193.56	Joback Method
cpg	1685.51	J/mol×K	1232.26	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=R59111&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R59111&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>
<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>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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