

# Pentane, 1,5-bis(methylthio)-

<b>Other names:</b>	2,8-Dithianonane
<b>Inchi:</b>	InChI=1S/C7H16S2/c1-8-6-4-3-5-7-9-2/h3-7H2,1-2H3
<b>InchiKey:</b>	AHJYQSDQHJYGCV-UHFFFAOYSA-N
<b>Formula:</b>	C7H16S2
<b>SMILES:</b>	CSCCCCCSC
<b>Mol. weight [g/mol]:</b>	164.33
<b>CAS:</b>	54410-63-8

## Physical Properties

Property code	Value	Unit	Source
gf	74.30	kJ/mol	Joback Method
hf	-104.07	kJ/mol	Joback Method
hfus	22.15	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.883		Crippen Method
mcvol	142.190	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	1339.00		NIST Webbook
tb	497.12	K	Joback Method
tc	706.23	K	Joback Method
tf	237.45	K	Joback Method
vc	0.535	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.36	J/molxK	497.12	Joback Method
cpg	309.83	J/molxK	531.97	Joback Method
cpg	322.69	J/molxK	566.82	Joback Method
cpg	334.95	J/molxK	601.67	Joback Method
cpg	346.61	J/molxK	636.52	Joback Method
cpg	357.67	J/molxK	671.38	Joback Method
cpg	368.15	J/molxK	706.23	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=C54410638&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54410638&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>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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