

# 3-propyl-2,4-dithiapentane

<b>Inchi:</b>	InChI=1S/C6H14S2/c1-4-5-6(7-2)8-3/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	NOCYIUVTTOGLND-UHFFFAOYSA-N
<b>Formula:</b>	C6H14S2
<b>SMILES:</b>	CCCC(SC)SC
<b>Mol. weight [g/mol]:</b>	150.31

## Physical Properties

Property code	Value	Unit	Source
gf	63.44	kJ/mol	Joback Method
hf	-88.71	kJ/mol	Joback Method
hfus	16.03	kJ/mol	Joback Method
hvap	42.20	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.839		Crippen Method
mvol	128.100	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1124.00		NIST Webbook
tb	473.80	K	Joback Method
tc	691.06	K	Joback Method
tf	211.18	K	Joback Method
vc	0.473	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.21	J/mol×K	473.80	Joback Method
cpg	266.88	J/mol×K	510.01	Joback Method
cpg	278.98	J/mol×K	546.22	Joback Method
cpg	290.51	J/mol×K	582.43	Joback Method
cpg	301.47	J/mol×K	618.64	Joback Method
cpg	311.87	J/mol×K	654.85	Joback Method
cpg	321.69	J/mol×K	691.06	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=R156788&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R156788&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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