

# Disulfide, ethyl 2-methylpropyl

<b>Other names:</b>	Ethyl isobutyl disulfide 2-Methyl-4,5-dithiaheptane Isobutyl ethyl disulfide Disulfide, ethyl isobutyl 6-Methyl-3,4-dithiaheptane
<b>Inchi:</b>	InChI=1S/C6H14S2/c1-4-7-8-5-6(2)3/h6H,4-5H2,1-3H3
<b>InchiKey:</b>	UMASWDYQHOTZKK-UHFFFAOYSA-N
<b>Formula:</b>	C6H14S2
<b>SMILES:</b>	CCSSCC(C)C
<b>Mol. weight [g/mol]:</b>	150.31
<b>CAS:</b>	40136-66-1

## 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	-2.85		Crippen Method
logp	3.044		Crippen Method
mcvol	128.100	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpol	1104.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1075.00		NIST Webbook
ripol	1363.00		NIST Webbook
tb	457.00 ± 1.70	K	NIST Webbook
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
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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>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C40136661&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C40136661&amp;Units=SI</a>
<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>

## 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>ripol:</b>	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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