

# trans-3-Methylcyclohexane-1-thiol

Inchi:	InChI=1S/C7H14S/c1-6-3-2-4-7(8)5-6/h6-8H,2-5H2,1H3/t6-,7+/m0/s1
InchiKey:	PWHHTYJQSMOEC-NKWVEPMBSA-N
Formula:	C7H14S
SMILES:	CC1CCCC(S)C1
Mol. weight [g/mol]:	130.25

## Physical Properties

Property code	Value	Unit	Source
gf	54.19	kJ/mol	Joback Method
hf	-115.35	kJ/mol	Joback Method
hfus	10.83	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.495		Crippen Method
mvol	114.980	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
tb	437.30	K	Joback Method
tc	666.53	K	Joback Method
tf	208.25	K	Joback Method
vc	0.413	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.46	J/mol×K	437.30	Joback Method
cpg	243.00	J/mol×K	475.50	Joback Method
cpg	259.60	J/mol×K	513.71	Joback Method
cpg	275.28	J/mol×K	551.91	Joback Method
cpg	290.07	J/mol×K	590.12	Joback Method
cpg	303.98	J/mol×K	628.32	Joback Method
cpg	317.03	J/mol×K	666.53	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=R524240&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R524240&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</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

Latest version available from:

<https://www.cheméo.com/cid/57-243-9/trans-3-Methylcyclohexane-1-thiol.pdf>

Generated by Cheméo on 2024-04-26 21:40:20.091301818 +0000 UTC m=+16456869.011879134.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.