

# cis,trans-2-Methyl-1-thiadecalin

<b>Other names:</b>	Cis-3-methyl-trans-2-thiabicyclo[4.4.0]decane
<b>Inchi:</b>	InChI=1S/C12H22S/c1-10-6-9-11(2)7-4-5-8-12(11,3)13-10/h10H,4-9H2,1-3H3/t10-,11-,12-
<b>InchiKey:</b>	YSNQSSXOPDJTBK-UTUOFQBUSA-N
<b>Formula:</b>	C10H18S
<b>SMILES:</b>	CC1CCC2(C)CCCC2(C)S1
<b>Mol. weight [g/mol]:</b>	170.31
<b>CAS:</b>	42900-30-1

## Physical Properties

Property code	Value	Unit	Source
gf	144.43	kJ/mol	Joback Method
hf	-114.65	kJ/mol	Joback Method
hfus	6.84	kJ/mol	Joback Method
hvap	46.02	kJ/mol	Joback Method
ie	7.80 ± 0.01	eV	NIST Webbook
log10ws	-4.50		Crippen Method
logp	4.241		Crippen Method
mcvol	174.570	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
tb	548.16	K	Joback Method
tc	795.75	K	Joback Method
tf	373.81	K	Joback Method
vc	0.630	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.64	J/mol×K	548.16	Joback Method
cpg	462.07	J/mol×K	589.43	Joback Method
cpg	483.74	J/mol×K	630.69	Joback Method
cpg	503.96	J/mol×K	671.96	Joback Method
cpg	523.08	J/mol×K	713.22	Joback Method
cpg	541.42	J/mol×K	754.49	Joback Method
cpg	559.31	J/mol×K	795.75	Joback Method

# Sources

<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=C42900301&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C42900301&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>

# 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>ie:</b>	Ionization energy
<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>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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