

# Tert-dodecyl mercaptan

<b>Other names:</b>	Decanethiol, 9,9-dimethyl-
<b>Inchi:</b>	InChI=1S/C12H26S/c1-12(2,3)10-8-6-4-5-7-9-11-13/h13H,4-11H2,1-3H3
<b>InchiKey:</b>	UVXGZLRXSOTRRS-UHFFFAOYSA-N
<b>Formula:</b>	C12H26S
<b>SMILES:</b>	CC(C)(C)CCCCCCCCS
<b>Mol. weight [g/mol]:</b>	202.40
<b>CAS:</b>	7341-22-2

## Physical Properties

Property code	Value	Unit	Source
gf	82.39	kJ/mol	Joback Method
hf	-261.28	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	47.75	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.693		Crippen Method
mcvol	196.290	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
tb	533.59	K	Joback Method
tc	722.19	K	Joback Method
tf	263.88	K	Joback Method
vc	0.750	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.83	J/mol×K	533.59	Joback Method
cpg	490.12	J/mol×K	565.02	Joback Method
cpg	507.49	J/mol×K	596.46	Joback Method
cpg	523.96	J/mol×K	627.89	Joback Method
cpg	539.59	J/mol×K	659.32	Joback Method
cpg	554.41	J/mol×K	690.75	Joback Method
cpg	568.46	J/mol×K	722.19	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=C7341222&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7341222&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>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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