

# 2-Undecanethiol, 2-methyl-

<b>Other names:</b>	1,1-Dimethyl-decyl-mercaptan 2-Methyl-2-undecanethiol 2-Methylundecane-2-thiol 2-Methylundecyl-2-thiol
<b>Inchi:</b>	InChI=1S/C12H26S/c1-4-5-6-7-8-9-10-11-12(2,3)13/h13H,4-11H2,1-3H3
<b>InchiKey:</b>	FRQQKWGDKVGLFI-UHFFFAOYSA-N
<b>Formula:</b>	C12H26S
<b>SMILES:</b>	CCCCCCCCCC(C)(C)S
<b>Mol. weight [g/mol]:</b>	202.40
<b>CAS:</b>	10059-13-9

## 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	-5.03		Crippen Method
logp	4.835		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	m3/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

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{\text{vp}}) = A + B/(T + C)$
Coeff. A	1.40041e+01
Coeff. B	-4.28724e+03
Coeff. C	-8.69190e+01
Temperature range (K), min.	399.48
Temperature range (K), max.	580.12

## 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=C10059139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10059139&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>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>pvap:</b>	Vapor 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

Latest version available from:

<https://www.chemeo.com/cid/67-567-9/2-Undecanethiol-2-methyl.pdf>

Generated by Cheméo on 2024-04-09 17:38:36.148382184 +0000 UTC m=+14973565.068959496.

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