

# 1-Decanethiol

<b>Other names:</b>	1-Decylthiol 1-MERCAPTODECANE DECANETHIOL-(1) Decyl mercaptan decane-1-thiol n-Decyl mercaptan
<b>Inchi:</b>	InChI=1S/C10H22S/c1-2-3-4-5-6-7-8-9-10-11/h11H,2-10H2,1H3
<b>InchiKey:</b>	VTXVGVNLYGSIAR-UHFFFAOYSA-N
<b>Formula:</b>	C10H22S
<b>SMILES:</b>	CCCCCCCCCS
<b>Mol. weight [g/mol]:</b>	174.35
<b>CAS:</b>	143-10-2

## Physical Properties

Property code	Value	Unit	Source
chl	-7405.10 ± 1.20	kJ/mol	NIST Webbook
gf	62.71	kJ/mol	Joback Method
hf	-211.90 ± 1.50	kJ/mol	NIST Webbook
hfl	-276.40 ± 1.40	kJ/mol	NIST Webbook
hfus	25.70	kJ/mol	Joback Method
hvap	65.48 ± 0.54	kJ/mol	NIST Webbook
hvap	65.48	kJ/mol	NIST Webbook
hvap	64.50 ± 0.40	kJ/mol	NIST Webbook
hvap	65.50 ± 0.50	kJ/mol	NIST Webbook
hvap	64.50	kJ/mol	NIST Webbook
log10ws	-4.08		Crippen Method
logp	4.057		Crippen Method
mvol	168.110	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1323.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1324.00		NIST Webbook
rinpol	1320.00		NIST Webbook
ripol	1571.00		NIST Webbook

ripol	1571.00		NIST Webbook
sl	476.13	J/molxK	NIST Webbook
tb	491.06	K	Joback Method
tc	673.00	K	Joback Method
tf	238.92	K	Joback Method
tt	247.87 ± 0.02	K	NIST Webbook
tt	247.85 ± 0.01	K	NIST Webbook
tt	247.87 ± 0.02	K	NIST Webbook
tt	247.85 ± 0.01	K	NIST Webbook
vc	0.649	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.06	J/molxK	612.35	Joback Method
cpg	445.22	J/molxK	642.67	Joback Method
cpg	373.06	J/molxK	491.06	Joback Method
cpg	388.80	J/molxK	521.38	Joback Method
cpg	403.87	J/molxK	551.71	Joback Method
cpg	418.28	J/molxK	582.03	Joback Method
cpg	457.79	J/molxK	673.00	Joback Method
cpl	350.41	J/molxK	298.15	NIST Webbook
cpl	349.63	J/molxK	298.15	NIST Webbook
cpl	365.44	J/molxK	300.00	NIST Webbook
hfust	33.30	kJ/mol	247.90	NIST Webbook
hfust	33.32	kJ/mol	247.86	NIST Webbook
hfust	33.32	kJ/mol	247.86	NIST Webbook
hfust	33.30	kJ/mol	247.90	NIST Webbook
hvapt	54.60	kJ/mol	473.50	NIST Webbook
hvapt	58.60	kJ/mol	288.00	NIST Webbook
hvapt	56.40	kJ/mol	467.00	NIST Webbook
sfust	134.42	J/molxK	247.86	NIST Webbook
sfust	134.42	J/molxK	247.86	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	1.70	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58516e+01
Coeff. B	-4.77343e+03
Coeff. C	-8.35830e+01
Temperature range (K), min.	390.28
Temperature range (K), max.	536.47

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.53103e+02
Coeff. B	-1.35869e+04
Coeff. C	-1.99591e+01
Coeff. D	9.74603e-06
Temperature range (K), min.	247.56
Temperature range (K), max.	696.00

# 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>KDB:</b>	<a href="https://www.thermo.com/files/research/kdb/mol/mol1848.mol">https://www.thermo.com/files/research/kdb/mol/mol1848.mol</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=C143102&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C143102&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>KDB Vapor Pressure Data:</b>	<a href="https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1848">https://www.thermo.com/research/kdb/hcprop/showprop.php?cmpid=1848</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>

# Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cpl:</b>	Liquid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>sl:</b>	Liquid phase molar entropy at standard conditions
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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