

# Heptadecyl mercaptan

<b>Other names:</b>	1-Heptadecanethiol
<b>Inchi:</b>	InChI=1S/C17H36S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h18H,2-17H2,1H3
<b>InchiKey:</b>	FXOGYMXDUYOYKR-UHFFFAOYSA-N
<b>Formula:</b>	C17H36S
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCCS
<b>Mol. weight [g/mol]:</b>	272.53
<b>CAS:</b>	53193-22-9

## Physical Properties

Property code	Value	Unit	Source
gf	121.65	kJ/mol	Joback Method
hf	-355.73	kJ/mol	Joback Method
hfus	43.83	kJ/mol	Joback Method
hvap	60.17	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	6.788		Crippen Method
mcvol	266.740	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
tb	651.22	K	Joback Method
tc	824.05	K	Joback Method
tf	317.81	K	Joback Method
vc	1.042	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.03	J/mol×K	651.22	Joback Method
cpg	756.57	J/mol×K	680.02	Joback Method
cpg	775.25	J/mol×K	708.83	Joback Method
cpg	793.08	J/mol×K	737.63	Joback Method
cpg	810.10	J/mol×K	766.44	Joback Method
cpg	826.35	J/mol×K	795.24	Joback Method
cpg	841.84	J/mol×K	824.05	Joback Method

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57510e+01
Coeff. B	-5.62086e+03
Coeff. C	-1.13832e+02
Temperature range (K), min.	477.33
Temperature range (K), max.	652.26

## Sources

<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>
<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=C53193229&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53193229&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>

## 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

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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