

# N-(2-octanoylmercapto) ethyloctanamide

Inchi:	InChI=1S/C18H35NO2S/c1-3-5-7-9-11-13-17(20)19-15-16-22-18(21)14-12-10-8-6-4-2/h3
InchiKey:	VHRMFSXVENWLHR-UHFFFAOYSA-N
Formula:	C18H35NO2S
SMILES:	CCCCCCCC(=O)SCCN=C(O)CCCCCC
Mol. weight [g/mol]:	329.54
CAS:	116401-75-3

## Physical Properties

Property code	Value	Unit	Source
hf	-565.36	kJ/mol	Joback Method
hvap	89.30	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.924		Crippen Method
mcvol	293.950	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
tb	902.63	K	Joback Method
tc	1106.17	K	Joback Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401753&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## Legend

**hf:** Enthalpy of formation at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

**log10ws:** 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

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<https://www.chemeo.com/cid/97-421-7/N-2-octanoylmercapto-ethyloctanamide.pdf>

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