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)CCCCCCC
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

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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature