Hexane, 1-(ethylthio)-

Other names:	1-(Ethylsulfanyl)hexane
	3-Thianonane
	Ethyl hexyl sulfide
	Hexyl ethyl sulfide
	Sulfide, ethyl hexyl
Inchi:	InChI=1S/C8H18S/c1-3-5-6-7-8-9-4-2/h3-8H2,1-2H3
InchiKey:	MGVUJBCOCITTRS-UHFFFAOYSA-N
Formula:	C8H18S
SMILES:	CCCCCCSCC
Mol. weight [g/mol]:	146.29
CAS:	7309-44-6

Physical Properties

Property code	Value	Unit	Source
gf	49.60	kJ/mol	Joback Method
hf	-166.58	kJ/mol	Joback Method
hfus	20.61	kJ/mol	Joback Method
hvap	40.22	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	3.320		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1092.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1092.00		NIST Webbook
ripol	1291.20		NIST Webbook
ripol	1291.20		NIST Webbook
ripol	1311.00		NIST Webbook
ripol	1286.60		NIST Webbook
tb	451.22	K	Joback Method
tc	636.81	K	Joback Method
tf	214.32	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.95	J/mol×K	451.22	Joback Method
cpg	300.83	J/mol×K	482.15	Joback Method
cpg	314.15	J/mol×K	513.08	Joback Method
cpg	326.93	J/mol×K	544.01	Joback Method
cpg	339.17	J/mol×K	574.95	Joback Method
cpg	350.89	J/mol×K	605.88	Joback Method
cpg	362.10	J/mol×K	636.81	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60224e+01
Coeff. B	-4.33235e+03
Coeff. C	-6.92250e+01
Temperature range (K), min.	344.56
Temperature range (K), max.	473.70

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C7309446&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume