1-Hexanethiol

Other names:	1-Hexylthiol
	Hexan-1-thiol
	Hexanethiol
	Hexyl mercaptan
	N-HEXYL MERCAPTAN
	N-HEXYLTHIOL
	USAF EK-4628
	hexane-1-thiol
	n-Hexanethiol
Inchi:	InChI=1S/C6H14S/c1-2-3-4-5-6-7/h7H,2-6H2,1H3
InchiKey:	PMBXCGGQNSVESQ-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CCCCCCS
Mol. weight [g/mol]:	118.24
CAS:	111-31-9

Physical Properties

Property code	Value	Unit	Source
chl	-4788.50 ± 0.75	kJ/mol	NIST Webbook
gf	29.03	kJ/mol	Joback Method
hf	-129.30 ± 0.96	kJ/mol	NIST Webbook
hfl	-175.70 ± 0.92	kJ/mol	NIST Webbook
hfus	15.34	kJ/mol	Joback Method
hvap	44.80 ± 0.20	kJ/mol	NIST Webbook
hvap	46.40	kJ/mol	NIST Webbook
log10ws	-2.41		Crippen Method
logp	2.497		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
rinpol	912.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	903.00		NIST Webbook
rinpol	920.00		NIST Webbook
rinpol	916.00		NIST Webbook

rinpol	921.00		NIST Webbook
rinpol	920.90		NIST Webbook
rinpol	927.30		NIST Webbook
rinpol	912.50		NIST Webbook
rinpol	916.40		NIST Webbook
rinpol	920.40		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	930.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	930.00		NIST Webbook
ripol	1148.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1153.20		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1145.00		NIST Webbook
ripol	1165.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1153.20		NIST Webbook
sl	343.21	J/mol×K	NIST Webbook
tb	422.85	K	KDB
tb	424.20	K	NIST Webbook
tb	425.75 ± 0.20	K	NIST Webbook
tb	420.00 ± 2.00	K	NIST Webbook
tc	588.15	K	Joback Method
tf	192.66 ± 0.02	K	NIST Webbook
tf	192.12 ± 0.30	K	NIST Webbook
tf	192.20 ± 0.30	K	NIST Webbook
tt	192.62 ± 0.02	K	NIST Webbook
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	257.60	J/mol×K	556.72	Joback Method
cpg	204.81	J/mol×K	399.54	Joback Method
cpg	216.29	J/mol×K	430.98	Joback Method
cpg	227.30	J/mol×K	462.41	Joback Method
cpg	237.85	J/mol×K	493.85	Joback Method
cpg	247.94	J/mol×K	525.28	Joback Method
cpg	266.84	J/mol×K	588.15	Joback Method
cpl	230.71	J/mol×K	298.15	NIST Webbook
cpl	230.68	J/mol×K	298.15	NIST Webbook
hfust	18.03	kJ/mol	192.60	NIST Webbook
hfust	18.01	kJ/mol	192.62	NIST Webbook
hfust	18.03	kJ/mol	192.60	NIST Webbook
hvapt	42.40	kJ/mol	410.00	NIST Webbook
hvapt	43.90	kJ/mol	387.00	NIST Webbook
sfust	93.51	J/mol×K	192.62	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55981e+01
Coeff. B	-4.00405e+03
Coeff. C	-5.95250e+01
Temperature range (K), min.	321.05
Temperature range (K), max.	448.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.11148e+01
Coeff. B	-8.11731e+03
Coeff. C	-9.63481e+00
Coeff. D	4.93320e-06
Temperature range (K), min.	192.62
Temperature range (K), max.	623.00

Sources

KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1834
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1834.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111319&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume