1-Propanethiol, 2-methyl-

Other names:	1-ISOBUTANETHIOL
	2-Methyl propanethiol
	2-Methyl-1-propanethiol
	2-Methyl-1-propylthiol
	2-methylpropane-1-thiol
	ISOBUTYL MERCAPTAN
	Isobutanethiol
	iso-C4H9SH
Inchi:	InChI=1S/C4H10S/c1-4(2)3-5/h4-5H,3H2,1-2H3
InchiKey:	BDFAOUQQXJIZDG-UHFFFAOYSA-N
Formula:	C4H10S
SMILES:	CC(C)CS
Mol. weight [g/mol]:	90.19
CAS:	513-44-0

Physical Properties

Property code	Value	Unit	Source
affp	802.60	kJ/mol	NIST Webbook
basg	771.40	kJ/mol	NIST Webbook
chl	-3473.50 ± 0.71	kJ/mol	NIST Webbook
gf	9.75	kJ/mol	Joback Method
hf	-96.48 ± 0.88	kJ/mol	NIST Webbook
hfl	-132.00 ± 0.88	kJ/mol	NIST Webbook
hfus	6.63	kJ/mol	Joback Method
hvap	34.70	kJ/mol	NIST Webbook
hvap	35.50	kJ/mol	NIST Webbook
hvap	34.70 ± 0.08	kJ/mol	NIST Webbook
hvap	34.60	kJ/mol	NIST Webbook
hvap	34.71	kJ/mol	NIST Webbook
ie	9.12	eV	NIST Webbook
log10ws	-1.33		Crippen Method
logp	1.572		Crippen Method
mcvol	83.570	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
rinpol	680.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	694.00		NIST Webbook

rinpol	658.00		NIST Webbook
rinpol	683.00		NIST Webbook
rinpol	641.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	687.80		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	680.10		NIST Webbook
rinpol	683.40		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	658.00		NIST Webbook
rinpol	660.00		NIST Webbook
rinpol	691.00		NIST Webbook
rinpol	688.00		NIST Webbook
rinpol	660.00		NIST Webbook
ripol	889.00		NIST Webbook
ripol	901.00		NIST Webbook
ripol	901.00		NIST Webbook
ripol	901.00		NIST Webbook
ripol	910.00		NIST Webbook
sl	266.35	J/mol×K	NIST Webbook
tb	314.35	K	KDB
tc	559.50	K	NIST Webbook
tf	128.30	K	KDB
tf	128.29 ± 0.02	K	NIST Webbook
tt	128.31 ± 0.05	K	NIST Webbook
vc	0.307	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.11	J/mol×K	548.81	Joback Method
cpg	143.11	J/mol×K	385.92	Joback Method
cpg	151.61	J/mol×K	418.50	Joback Method
cpg	159.74	J/mol×K	451.07	Joback Method
cpg	167.54	J/mol×K	483.65	Joback Method
cpg	174.99	J/mol×K	516.23	Joback Method
cpg	134.26	J/mol×K	353.34	Joback Method
cpl	171.88	J/mol×K	298.15	NIST Webbook
hfust	4.98	kJ/mol	128.30	NIST Webbook

hfust	4.98	kJ/mol	128.30	NIST Webbook
hfust	4.98	kJ/mol	128.31	NIST Webbook
hvapt	31.01	kJ/mol	361.60	NIST Webbook
hvapt	33.60	kJ/mol	356.50	NIST Webbook
hvapt	33.30 ± 0.10	kJ/mol	321.00	NIST Webbook
hvapt	32.30 ± 0.10	kJ/mol	340.00	NIST Webbook
hvapt	31.00 ± 0.10	kJ/mol	361.00	NIST Webbook
sfust	388.30	J/mol×K	128.31	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54360e+01
Coeff. B	-3.45422e+03
Coeff. C	-4.16860e+01
Temperature range (K), min.	269.71
Temperature range (K), max.	382.86

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.91856e+01
Coeff. B	-6.70084e+03
Coeff. C	-9.67807e+00
Coeff. D	7.43090e-06
Temperature range (K), min.	128.31
Temperature range (K), max.	559.00

Sources

Measurement of Henry s Law constant and infinite dilution activity coefficient of isopropyl mercaptan and isobutyl mercaptan in (methyldiethanolamine (1) + water (2)) with w1 = 0.25 and 0.50 at temperature of (298 to 348) K using inert gas stripping method:	https://www.doi.org/10.1016/j.jct.2015.10.005
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1820
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C513440&Units=SI
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1820.mol

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
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

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