2-Propanethiol, 2-methyl-

Other names:	1,1-Dimethylethanethiol
	2-Isobutanethiol
	2-Methyl-2-propanethiol
	2-Methyl-2-propylthiol
	2-methylpropane-2-thiol
	TERT-BUTYL MERCAPTAN
	TERT-BUTYLTHIOL
	t-Butyl mercaptan
	tert-Butanethiol
	tert-Butyl hydrosulfide
	tert-Butylmercaptan
	tert-C4H9SH
	tertiary-Butyl mercaptan
Inchi:	InChI=1S/C4H10S/c1-4(2,3)5/h5H,1-3H3
InchiKey:	WMXCDAVJEZZYLT-UHFFFAOYSA-N
Formula:	C4H10S
SMILES:	CC(C)(C)S
Mol. weight [g/mol]:	90.19
CAS:	75-66-1

Physical Properties

Property code	Value	Unit	Source
affp	816.40	kJ/mol	NIST Webbook
basg	785.10	kJ/mol	NIST Webbook
chl	-3465.00 ± 0.71	kJ/mol	NIST Webbook
gf	15.03	kJ/mol	Joback Method
hf	-108.70 ± 0.88	kJ/mol	NIST Webbook
hfl	-140.50 ± 0.88	kJ/mol	NIST Webbook
hfus	2.74	kJ/mol	Joback Method
hvap	31.80	kJ/mol	NIST Webbook
hvap	30.93	kJ/mol	NIST Webbook
hvap	30.80	kJ/mol	NIST Webbook
hvap	30.90 ± 0.08	kJ/mol	NIST Webbook
ie	9.03	eV	NIST Webbook
log10ws	-1.68		Crippen Method
logp	1.715		Crippen Method
mcvol	83.570	ml/mol	McGowan Method

pc	4333.96	kPa	Joback Method
rinpol	599.20		NIST Webbook
rinpol	602.50		NIST Webbook
rinpol	617.00		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	574.00		NIST Webbook
rinpol	577.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	599.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	605.50		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	589.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	584.00		NIST Webbook
ripol	779.00		NIST Webbook
ripol	779.00		NIST Webbook
sl	246.44	J/mol×K	NIST Webbook
tb	337.40	K	NIST Webbook
tb	334.75	K	KDB
tb	337.00 ± 2.00	K	NIST Webbook
tb	337.90 ± 0.60	K	NIST Webbook
tb	334.50 ± 0.35	K	NIST Webbook
tb	336.00 ± 3.00	K	NIST Webbook
tb	337.40	K	NIST Webbook
tb	337.00	K	NIST Webbook
tb	339.00 ± 2.00	K	NIST Webbook
tc	530.10	K	NIST Webbook
tf	273.97 ± 0.20	K	NIST Webbook
tf	274.41	K	KDB
tt	274.42 ± 0.02	K	NIST Webbook
vc	0.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.83	J/mol×K	452.80	Joback Method
cpg	180.21	J/mol×K	520.97	Joback Method
cpg	172.28	J/mol×K	486.88	Joback Method
cpg	135.13	J/mol×K	350.55	Joback Method
cpg	145.28	J/mol×K	384.63	Joback Method
cpg	154.84	J/mol×K	418.72	Joback Method
cpg	187.65	J/mol×K	555.05	Joback Method
cpl	175.06	J/mol×K	298.15	NIST Webbook
hfust	0.97	kJ/mol	199.40	NIST Webbook
hfust	0.65	kJ/mol	157.00	NIST Webbook
hfust	4.07	kJ/mol	151.60	NIST Webbook
hfust	2.48	kJ/mol	274.40	NIST Webbook
hfust	2.48	kJ/mol	274.40	NIST Webbook
hvapt	30.90	kJ/mol	333.00	NIST Webbook
hvapt	30.10	kJ/mol	284.00	NIST Webbook
hvapt	28.45	kJ/mol	337.40	NIST Webbook
rfi	1.42000		293.10	Isothermal Binary Vapor-Liquid Equilibrium for 2-Methylpropane and n-Butane with 1,2-Ethanedithiol and 2-Methyl-2-propanethiol
rfi	1.42000		298.15	Vapor Liquid Equilibrium for Methoxymethane + Thiophene, + Diethylsulfide, + 2-Methyl-2-propanethiol and 1-Hexene, + 1-Propanethiol
sfust	26.83	J/mol×K	151.60	NIST Webbook
sfust	9.04	J/mol×K	274.40	NIST Webbook
sfust	4.87	J/mol×K	199.40	NIST Webbook
sfust	4.13	J/mol×K	157.00	NIST Webbook

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1822.mol

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75661&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapor Liquid Equilibrium for Methoxymethane + Thiophene, + Diethylsulfide, + 2-Methylpropane and 1-Propanethiol and 1-Hexene, + 1-Propanethiol:	https://www.doi.org/10.1021/je3013028
Isothermal Binary Vapor-Liquid Equilibrium for 2-Methylpropane and 2-Methyl-2-propanethiol and 1-Hexene, + 1-Propanethiol:	https://www.doi.org/10.1021/je9003417
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rfi:	Refractive Index
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