2-Butanethiol, 2-methyl-

Other names:	1,1-Dimethyl-1-propanethiol
	1,1-diMethyl-1-Propylthiol
	2-METHYLBUTANE-2-THIOL
	2-Methybutane-2-thiol
	2-Methyl-2-butanethiol
	2-Methylbutan-2-thiol
	2-tert-Pentyl mercaptan
	TERT-AMYL MERCAPTAN
	TERT-PENTYL MERCAPTAN
Inchi:	InChI=1S/C5H12S/c1-4-5(2,3)6/h6H,4H2,1-3H3
InchiKey:	IQIBYAHJXQVQGB-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCC(C)(C)S
Mol. weight [g/mol]:	104.21
CAS:	1679-09-0

Physical Properties

Property code	Value	Unit	Source
chl	-4122.00 ± 0.79	kJ/mol	NIST Webbook
gf	23.45	kJ/mol	Joback Method
hf	-126.90 ± 0.92	kJ/mol	NIST Webbook
hfl	-162.60 ± 0.88	kJ/mol	NIST Webbook
hfus	5.33	kJ/mol	Joback Method
hvap	35.70	kJ/mol	NIST Webbook
hvap	35.70	kJ/mol	NIST Webbook
hvap	35.60	kJ/mol	NIST Webbook
hvap	35.73	kJ/mol	NIST Webbook
log10ws	-2.10		Crippen Method
logp	2.105		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
rinpol	728.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	728.00		NIST Webbook
ripol	918.00		NIST Webbook

sl	290.12	J/mol×K	NIST Webbook
tb	372.35 ± 0.20	K	NIST Webbook
tb	372.70	K	NIST Webbook
tb	375.20	K	NIST Webbook
tb	372.30	K	NIST Webbook
tc	570.10	K	NIST Webbook
tf	184.99	K	Joback Method
tt	169.30 ± 0.20	K	NIST Webbook
tt	169.25 ± 0.20	K	NIST Webbook
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.27	J/mol×K	407.32	Joback Method
cpg	192.27	J/mol×K	441.20	Joback Method
cpg	169.61	J/mol×K	373.43	Joback Method
cpg	230.22	J/mol×K	576.75	Joback Method
cpg	221.58	J/mol×K	542.86	Joback Method
cpg	212.39	J/mol×K	508.98	Joback Method
cpg	202.63	J/mol×K	475.09	Joback Method
cpl	198.15	J/mol×K	298.15	NIST Webbook
hfust	7.06	kJ/mol	144.50	NIST Webbook
hfust	0.61	kJ/mol	146.10	NIST Webbook
hvapt	36.30	kJ/mol	337.00	NIST Webbook
hvapt	31.37	kJ/mol	372.30	NIST Webbook
hvapt	31.40 ± 0.10	kJ/mol	372.00	NIST Webbook
hvapt	32.70 ± 0.10	kJ/mol	350.00	NIST Webbook
hvapt	33.80 ± 0.10	kJ/mol	330.00	NIST Webbook
hvapt	34.30	kJ/mol	365.50	NIST Webbook
sfust	4.15	J/mol×K	146.10	NIST Webbook
sfust	48.87	J/mol×K	144.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.50495e+01
Coeff. B	-3.44809e+03
Coeff. C	-4.46440e+01
Temperature range (K), min.	278.22
Temperature range (K), max.	398.73

Sources

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/mol1829.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1679090&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