1-Butanethiol, 2-methyl-

Other names:	2-Methyl-1-butanethiol
	2-Methylbutan-1-thiol
	2-methylbutane-1-thiol
	CH3CH2CH(CH3)CH2SH
Inchi:	InChI=1S/C5H12S/c1-3-5(2)4-6/h5-6H,3-4H2,1-2H3
InchiKey:	WGQKBCSACFQGQY-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CCC(C)CS
Mol. weight [g/mol]:	104.21
CAS:	1878-18-8

Physical Properties

Property code	Value	Unit	Source
chl	-4130.40 ± 0.84	kJ/mol	NIST Webbook
gf	18.17	kJ/mol	Joback Method
hf	-114.70 ± 0.96	kJ/mol	NIST Webbook
hfl	-154.10 ± 0.92	kJ/mol	NIST Webbook
hfus	9.22	kJ/mol	Joback Method
hvap	39.70	kJ/mol	NIST Webbook
hvap	39.50	kJ/mol	NIST Webbook
hvap	39.40	kJ/mol	NIST Webbook
hvap	39.40 ± 0.20	kJ/mol	NIST Webbook
hvap	39.90 ± 0.10	kJ/mol	NIST Webbook
log10ws	-1.75		Crippen Method
logp	1.962		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
rinpol	771.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	775.00		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	1004.00		NIST Webbook
ripol	1004.00		NIST Webbook
tb	392.25 ± 0.20	K	NIST Webbook
tb	392.20	K	NIST Webbook
tb	389.70	K	NIST Webbook

tb	389.00 ± 2.50	K	NIST Webbook
tc	591.90	K	NIST Webbook
tf	167.57	K	Joback Method
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.28	J/mol×K	376.22	Joback Method
cpg	178.71	J/mol×K	408.64	Joback Method
cpg	188.71	J/mol×K	441.05	Joback Method
cpg	198.28	J/mol×K	473.47	Joback Method
cpg	207.43	J/mol×K	505.89	Joback Method
cpg	216.18	J/mol×K	538.31	Joback Method
cpg	224.53	J/mol×K	570.72	Joback Method
hvapt	33.79	kJ/mol	392.20	NIST Webbook
hvapt	39.20	kJ/mol	355.50	NIST Webbook
hvapt	37.60	kJ/mol	378.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56716e+01
Coeff. B	-3.75294e+03
Coeff. C	-5.01670e+01
Temperature range (K), min.	294.12
Temperature range (K), max.	412.42

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1878188&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume