2-Butanethiol, 3-methyl-

Other names:	3-Methyl-2-butanethiol
	3-Methyl-2-butylthiol
	3-Methylbutan-2-thiol
	3-methylbutane-2-thiol
Inchi:	InChI=1S/C5H12S/c1-4(2)5(3)6/h4-6H,1-3H3
InchiKey:	BFLXFRNPNMTTAA-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CC(C)C(C)S
Mol. weight [g/mol]:	104.21
CAS:	2084-18-6

Physical Properties

Property code	Value	Unit	Source
chl	-4126.00 ± 0.84	kJ/mol	NIST Webbook
gf	15.73	kJ/mol	Joback Method
hf	-121.00 ± 0.96	kJ/mol	NIST Webbook
hfl	-158.40 ± 0.92	kJ/mol	NIST Webbook
hfus	5.70	kJ/mol	Joback Method
hvap	37.50 ± 0.10	kJ/mol	NIST Webbook
hvap	37.70	kJ/mol	NIST Webbook
hvap	37.40	kJ/mol	NIST Webbook
hvap	37.50 ± 0.20	kJ/mol	NIST Webbook
log10ws	-1.86		Crippen Method
logp	1.961		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	773.00		NIST Webbook
rinpol	743.00		NIST Webbook
rinpol	773.00		NIST Webbook
ripol	978.00		NIST Webbook
sl	295.60	J/mol×K	NIST Webbook
tb	382.95 ± 0.20	K	NIST Webbook
tc	575.16	K	Joback Method
tf	152.57	K	Joback Method
tt	146.05 ± 0.06	K	NIST Webbook
vc	0.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.64	J/mol×K	508.70	Joback Method
cpg	226.21	J/mol×K	575.16	Joback Method
cpg	217.64	J/mol×K	541.93	Joback Method
cpg	168.20	J/mol×K	375.78	Joback Method
cpg	179.00	J/mol×K	409.01	Joback Method
cpg	189.33	J/mol×K	442.24	Joback Method
cpg	199.21	J/mol×K	475.47	Joback Method
cpl	198.95	J/mol×K	298.15	NIST Webbook
hfust	0.61	kJ/mol	146.10	NIST Webbook
hfust	0.61	kJ/mol	191.00	NIST Webbook
hfust	7.06	kJ/mol	144.50	NIST Webbook
hvapt	36.20	kJ/mol	368.50	NIST Webbook
hvapt	37.70	kJ/mol	347.00	NIST Webbook
sfust	4.16	J/mol×K	146.10	NIST Webbook
sfust	48.89	J/mol×K	144.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53811e+01
Coeff. B	-3.60930e+03
Coeff. C	-4.75990e+01
Temperature range (K), min.	286.73
Temperature range (K), max.	406.03

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2084186&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

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