1-Butanethiol, 3-methyl-

Other names:	2-Methyl-4-butanethiol
	3-Methyl-1-butanethiol
	3-Methyl-1-butylthiol
	3-Methylbutan-1-thiol
	3-Methylbutanethiol
	3-methylbutane-1-thiol
	Isoamyl mercaptan
	Isoamyl sulfhydrate
	Isopentyl mercaptan
Inchi:	InChI=1S/C5H12S/c1-5(2)3-4-6/h5-6H,3-4H2,1-2H3
InchiKey:	GIJGXNFNUUFEGH-UHFFFAOYSA-N
Formula:	C5H12S
SMILES:	CC(C)CCS
Mol. weight [g/mol]:	104.21
CAS:	541-31-1

Physical Properties

Property code	Value	Unit	Source
chl	-4130.50 ± 1.10	kJ/mol	NIST Webbook
gf	18.17	kJ/mol	Joback Method
hf	-114.60 ± 1.20	kJ/mol	NIST Webbook
hfl	-154.10 ± 1.20	kJ/mol	NIST Webbook
hfus	9.22	kJ/mol	Joback Method
hvap	39.40 ± 0.20	kJ/mol	NIST Webbook
hvap	39.70	kJ/mol	NIST Webbook
hvap	39.50	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	768.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	794.00		NIST Webbook
ripol	1017.00		NIST Webbook
ripol	1017.00		NIST Webbook

sl	298.49	J/mol×K	NIST Webbook
tb	391.20	K	NIST Webbook
tc	570.72	K	Joback Method
tf	167.57	K	Joback Method
tt	139.63 ± 0.01	K	NIST Webbook
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	188.71	J/mol×K	441.05	Joback Method
cpg	178.71	J/mol×K	408.64	Joback Method
cpg	224.53	J/mol×K	570.72	Joback Method
cpg	216.18	J/mol×K	538.31	Joback Method
cpg	207.43	J/mol×K	505.89	Joback Method
cpg	198.28	J/mol×K	473.47	Joback Method
cpg	168.28	J/mol×K	376.22	Joback Method
cpl	200.33	J/mol×K	298.15	NIST Webbook
cps	93.72	J/mol×K	103.00	NIST Webbook
hfust	7.41	kJ/mol	139.60	NIST Webbook
hfust	7.41	kJ/mol	139.60	NIST Webbook
hfust	7.41	kJ/mol	139.63	NIST Webbook
hvapt	37.70	kJ/mol	377.00	NIST Webbook
hvapt	39.30	kJ/mol	355.00	NIST Webbook
sfust	53.04	J/mol×K	139.63	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54274e+01
Coeff. B	-3.68822e+03
Coeff. C	-4.99860e+01
Temperature range (K), min.	293.60
Temperature range (K), max.	414.58

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=C541311&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
cps:	Solid 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

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