2-Butanethiol, 2,3-dimethyl-

Other names:	2,3-Dimethyl-2-butanethiol
Inchi:	InChI=1S/C6H14S/c1-5(2)6(3,4)7/h5,7H,1-4H3
InchiKey:	CRJLQECEGNIMNG-UHFFFAOYSA-N
Formula:	C6H14S
SMILES:	CC(C)C(C)(C)S
Mol. weight [g/mol]:	118.24
CAS:	1639-01-6

Physical Properties

Property code	Value	Unit	Source
chl	-4777.04 ± 0.67	kJ/mol	NIST Webbook
gf	29.43	kJ/mol	Joback Method
hf	-147.90 ± 1.00	kJ/mol	NIST Webbook
hfl	-187.20 ± 1.00	kJ/mol	NIST Webbook
hfus	4.40	kJ/mol	Joback Method
hvap	39.30 ± 0.10	kJ/mol	NIST Webbook
hvap	39.30 ± 0.20	kJ/mol	NIST Webbook
hvap	39.30	kJ/mol	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.351		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	801.00		NIST Webbook
tb	395.87	K	Joback Method
tc	602.65	K	Joback Method
tf	181.26	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.45	J/mol×K	395.87	Joback Method
cpg	219.89	J/mol×K	430.33	Joback Method
cpg	232.57	J/mol×K	464.80	Joback Method

cpg	244.51	J/mol×K	499.26	Joback Method
cpg	255.75	J/mol×K	533.72	Joback Method
cpg	266.33	J/mol×K	568.18	Joback Method
cpg	276.28	J/mol×K	602.65	Joback Method
hvapt	39.30	kJ/mol	301.50	NIST Webbook
hvapt	37.80	kJ/mol	379.50	NIST Webbook
hvapt	37.40	kJ/mol	384.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45703e+01
Coeff. B	-3.65498e+03
Coeff. C	-5.67450e+01
Temperature range (K), min.	312.65
Temperature range (K), max.	451.50

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=C1639016&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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