1,4-Butanedithiol

Other names:	1,4-Dimercaptobutane
	Tetramethylene dimercaptan
	Tetramethylenedithiol
	butane-1,4-dithiol
Inchi:	InChI=1S/C4H10S2/c5-3-1-2-4-6/h5-6H,1-4H2
InchiKey:	SMTOKHQOVJRXLK-UHFFFAOYSA-N
Formula:	C4H10S2
SMILES:	SCCCCS
Mol. weight [g/mol]:	122.25
CAS:	1191-08-8

Physical Properties

Property code	Value	Unit	Source
chl	-4102.20 ± 1.70	kJ/mol	NIST Webbook
gf	41.58	kJ/mol	Joback Method
hf	-50.50 ± 1.80	kJ/mol	NIST Webbook
hfl	-105.80 ± 1.80	kJ/mol	NIST Webbook
hfus	14.20	kJ/mol	Joback Method
hvap	55.30	kJ/mol	NIST Webbook
hvap	55.30	kJ/mol	NIST Webbook
hvap	55.10	kJ/mol	NIST Webbook
hvap	55.30 ± 0.40	kJ/mol	NIST Webbook
hvap	54.90	kJ/mol	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.626		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4602.62	kPa	Joback Method
rinpol	1063.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1063.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1574.00		NIST Webbook
tb	468.70	K	NIST Webbook
tc	634.88	K	Joback Method
tf	207.76	K	Joback Method

vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.16	J/mol×K	598.51	Joback Method
cpg	173.71	J/mol×K	416.64	Joback Method
cpg	183.09	J/mol×K	453.01	Joback Method
cpg	192.02	J/mol×K	489.39	Joback Method
cpg	200.49	J/mol×K	525.76	Joback Method
cpg	208.53	J/mol×K	562.14	Joback Method
cpg	223.37	J/mol×K	634.88	Joback Method
hvapt	50.90	kJ/mol	408.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42534e+01
Coeff. B	-3.76018e+03
Coeff. C	-7.84410e+01
Temperature range (K), min.	347.68
Temperature range (K), max.	498.95

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1191088&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume