1,3-Butanedithiol

Other names:	1,3-dimercaptobutane
	butane-1,3-dithiol
Inchi:	InChI=1S/C4H10S2/c1-4(6)2-3-5/h4-6H,2-3H2,1H3
InchiKey:	XMEPRJBZFCWFKN-UHFFFAOYSA-N
Formula:	C4H10S2
SMILES:	CC(S)CCS
Mol. weight [g/mol]:	122.25
CAS:	24330-52-7

Physical Properties

Property code	Value	Unit	Source
gf	39.14	kJ/mol	Joback Method
hf	-54.21	kJ/mol	Joback Method
hfus	10.68	kJ/mol	Joback Method
hvap	37.58	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.625		Crippen Method
mcvol	99.920	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
ripol	1456.00		NIST Webbook
tb	416.20	K	Joback Method
tc	639.97	K	Joback Method
tf	192.76	K	Joback Method
vc	0.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.79	J/mol×K	416.20	Joback Method
cpg	183.51	J/mol×K	453.50	Joback Method
cpg	192.74	J/mol×K	490.79	Joback Method
cpg	201.50	J/mol×K	528.09	Joback Method

cpg	209.78	J/mol×K	565.38	Joback Method
cpg	217.62	J/mol×K	602.68	Joback Method
cpg	225.02	J/mol×K	639.97	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35882e+01
Coeff. B	-3.60799e+03
Coeff. C	-6.86550e+01
Temperature range (K), min.	339.92
Temperature range (K), max.	504.58

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=C24330527&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

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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