2,3-Dimercaptopropan-1-ol

Other names:	1,2-Dimercapto-3-propanol
	1,2-Dithioglycerol
	1-Propanol, 2,3-dimercapto-
	2,3-Dimercapto-1-propanol
	2,3-Dimercaptol-1-propanol
	2,3-Dimercaptopropanol
	2,3-Dithiopropanol
	2,3-Mercaptopropan-1-ol
	3-Hydroxy-1,2-propanedithiol
	Antoxol
	BAL
	BAL in Oil
	British Anti-Lewisite
	DMP
	Dicaptol
	Dimercaprol
	Dimercaprol propanol
	Dimercaptopropanol
	Dimerkaprol
	Dimersol
	Dithioglycerine
	Dithioglycerol
	Glycerol, 1,2-dithio-
	NSC 39515
	NSC 4646
	Panobal
	Sulfactin
	USAF ME-1
	«alpha»,«beta»-Dithioglycerol
	Â«alphaÂ»,Â«betaÂ»-Dithioglycerol
Inchi:	InChI=1S/C3H8OS2/c4-1-3(6)2-5/h3-6H,1-2H2
InchiKey:	WQABCVAJNWAXTE-UHFFFAOYSA-N
Formula:	C3H8OS2
SMILES:	OCC(S)CS
Mol. weight [g/mol]:	124.22
CAS:	59-52-9

Physical Properties

Property code	Value	Unit	Source
gf	-106.10	kJ/mol	Joback Method
hf	-185.80	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	52.04	kJ/mol	Joback Method
log10ws	-0.60		Crippen Method
logp	0.207		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	6122.63	kPa	Joback Method
tb	485.50	K	Joback Method
tc	697.86	K	Joback Method
tf	242.31	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.46	J/mol×K	485.50	Joback Method
cpg	180.47	J/mol×K	520.89	Joback Method
cpg	187.12	J/mol×K	556.29	Joback Method
cpg	193.42	J/mol×K	591.68	Joback Method
cpg	199.36	J/mol×K	627.07	Joback Method
cpg	204.97	J/mol×K	662.46	Joback Method
cpg	210.26	J/mol×K	697.86	Joback Method
hvapt	61.20	kJ/mol	383.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.30344e+01
Coeff. B	-8.73316e+03
Temperature range (K), min.	353.00
Temperature range (K), max.	492.76

Sources

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=C59529&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

vc: Critical Volume

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