

1,4-Dithiothreitol

Other names:	Dithiothreitol
	1,4-Dithio-dl-threitol
	dl-Dithiothreitol
	2,3-Butanediol, 1,4-dimercapto-, (R*,R*)-(./-.)-
	Threitol, 1,4-dithio-, dl-
	2,3-Butanediol, 1,4-dimercapto-, dl, threo-
	Cleland's reagent
	DL-threo-1,4-Dimercapto-2,3-butanediol
	DL-1,4-Dithiothreitol
	rac-Dithiothreitol
	DTT
	1,4-Disulfanyl-2,3-butanediol, dl, threo-
	(./-.)-Dithiothreitol
	2,3-Butanediol, 1,4-dimercapto-, (2R,3R)-rel-
	Sputolysin
	Threitol, 1,4-dithio-
	WR 34678
	(R*,R*)-1,4-dimercaptobutane-2,3-diol
Inchi:	InChI=1S/C4H10O2S2/c5-3(1-7)4(6)2-8/h3-8H,1-2H2
InchiKey:	VHJLVAABSRFDPM-UHFFFAOYSA-N
Formula:	C4H10O2S2
SMILES:	OC(CS)C(O)CS
Mol. weight [g/mol]:	154.25
CAS:	3483-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-236.94	kJ/mol	Joback Method
hf	-363.95	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	70.55	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	-0.432		Crippen Method
mcvol	111.660	ml/mol	McGowan Method
pc	6161.14	kPa	Joback Method
tb	600.12	K	Joback Method

tc	799.63	K	Joback Method
tf	299.40	K	Joback Method
vc	0.394	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.41	J/mol×K	600.12	Joback Method
cpg	258.61	J/mol×K	633.37	Joback Method
cpg	265.41	J/mol×K	666.62	Joback Method
cpg	271.83	J/mol×K	699.87	Joback Method
cpg	277.88	J/mol×K	733.12	Joback Method
cpg	283.58	J/mol×K	766.38	Joback Method
cpg	288.94	J/mol×K	799.63	Joback Method

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=C3483123&Units=SI

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
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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