

S,S'-TETRAMETHYLENE BIS(METHANETHIOSULFONATE)

Other names:	1,4-Butanediol, S-dimethanethiosulfonate
Inchi:	InChI=1S/C6H14O4S4/c1-13(7,8)11-5-3-4-6-12-14(2,9)10/h3-6H2,1-2H3
InchiKey:	VIISOSSRZYEECK-UHFFFAOYSA-N
Formula:	C6H14O4S4
SMILES:	CS(=O)(=O)SCCCCSS(C)(=O)=O
Mol. weight [g/mol]:	278.44

Physical Properties

Property code	Value	Unit	Source
hfus	42.31	kJ/mol	Joback Method
logp	1.152		Crippen Method
mcvol	184.280	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.97	J/mol×K	569.80	Joback Method
cpg	423.12	J/mol×K	602.86	Joback Method
cpg	435.60	J/mol×K	635.92	Joback Method
cpg	447.36	J/mol×K	668.97	Joback Method
cpg	458.40	J/mol×K	702.03	Joback Method
cpg	468.68	J/mol×K	735.09	Joback Method
cpg	478.17	J/mol×K	768.15	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55992&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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