1,4-Benzenedithiol, S,S'-dimethyl-

Inchi: InChI=1S/C8H10S2/c1-9-7-3-5-8(10-2)6-4-7/h3-6H,1-2H3
InchiKey: CVZBYEKCIDMLRV-UHFFFAOYSA-N
Formula: C8H10S2
SMILES: CSc1ccc(SC)cc1
Mol. weight [g/mol]: 170.29

Physical Properties

Property code	Value	Unit	Source
gf	185.50	kJ/mol	Joback Method
hf	100.35	kJ/mol	Joback Method
hfus	18.39	kJ/mol	Joback Method
hvap	49.97	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	3.130		Crippen Method
mcvol	132.520	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	1559.40		NIST Webbook
rinpol	1559.40		NIST Webbook
tb	551.66	K	Joback Method
tc	810.58	K	Joback Method
tf	287.66	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	269.16	J/mol×K	551.66	Joback Method
cpg	282.32	J/mol×K	594.81	Joback Method
cpg	294.57	J/mol×K	637.97	Joback Method
cpg	305.93	J/mol×K	681.12	Joback Method
cpg	316.41	J/mol×K	724.28	Joback Method
cpg	326.03	J/mol×K	767.43	Joback Method
cpg	334.81	J/mol×K	810.58	Joback Method

Sources

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=U353072&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume