1,4-Dithiane, 3,6-dimethyl

Other names: 2,5-dimethyl-1,4-dithiane
1,4-Dithiacyclohexane, 3,6-dimethyl
1,4-Dithiane, 3,6-dimethyl
Inchi: InChI=1S/C6H12S2/c1-5-3-8-6(2)4-7-5/h5-6H,3-4H2,1-2H3
InchiKey: OGQAHQBLZPEVNY-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CC1CSC(C)CS1
Mol. weight [g/mol]: 148.30

Physical Properties

Property code	Value	Unit	Source
hf	-86.73	kJ/mol	Cheméo Relay (1.0)
hfus	11.52	kJ/mol	Joback Method
ie	8.43	eV	Cheméo Relay (1.0)
logp	2.243		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
rinpol	1157.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1130.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1584.00		NIST Webbook
tb	471.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.86	J/mol×K	447.22	Joback Method
cpg	241.60	J/mol×K	487.02	Joback Method

cpg	256.46	J/mol×K	526.83	Joback Method
cpg	270.45	J/mol×K	566.63	Joback Method
cpg	283.61	J/mol×K	606.43	Joback Method
cpg	295.94	J/mol×K	646.23	Joback Method
cpg	307.49	J/mol×K	686.04	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72033375&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
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature