3,6-dimethyl-1,4-dithiane

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]: 148.29
CAS: 72033-37-5

Physical Properties

Property code	Value	Unit	Source
gf	96.10	kJ/mol	Joback Method
hf	-42.67	kJ/mol	Joback Method
hfus	11.52	kJ/mol	Joback Method
hvap	40.69	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.243		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1157.00		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
rinpol	1137.00		NIST Webbook
ripol	1584.00		NIST Webbook
ripol	1584.00		NIST Webbook
tb	447.22	K	Joback Method
tc	686.04	K	Joback Method
tf	327.42	K	Joback Method
vc	0.396	m3/kmol	Joback Method

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

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=C72033375&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume