1,4-Dithiane, 3,5-dimethyl, #2

Inchi: InChI=1S/C6H12S2/c1-5-3-7-4-6(2)8-5/h5-6H,3-4H2,1-2H3
InchiKey: VUMHVPHHEVBMOI-UHFFFAOYSA-N
Formula: C6H12S2
SMILES: CC1CSCC(C)S1
Mol. weight [g/mol]: 148.29

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	1152.00		NIST Webbook
rinpol	1152.00		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=R82213&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