2,2-dimethyl-4,5-dithiaoctane

Inchi: InChI=1S/C8H18S2/c1-5-6-9-10-7-8(2,3)4/h5-7H2,1-4H3
InchiKey: BCWAUAWMZLMXSS-UHFFFAOYSA-N
Formula: C8H18S2
SMILES: CCCSSCC(C)(C)C
Mol. weight [g/mol]: 178.36

Physical Properties

Property code	Value	Unit	Source
gf	85.56	kJ/mol	Joback Method
hf	-133.46	kJ/mol	Joback Method
hfus	17.32	kJ/mol	Joback Method
hvap	45.74	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.824		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1225.00		NIST Webbook
rinpol	1225.00		NIST Webbook
tb	516.77	K	Joback Method
tc	736.19	K	Joback Method
tf	251.14	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.93	J/mol×K	516.77	Joback Method
cpg	359.54	J/mol×K	553.34	Joback Method
cpg	374.26	J/mol×K	589.91	Joback Method
cpg	388.10	J/mol×K	626.48	Joback Method
cpg	401.11	J/mol×K	663.05	Joback Method
cpg	413.31	J/mol×K	699.62	Joback Method
cpg	424.73	J/mol×K	736.19	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=R155403&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