dimethyl-1,2,3,6-tetrathiacyclooctane

Inchi: InChI=1S/C6H12S4/c1-5-3-7-10-8-4-6(2)9-5/h5-6H,3-4H2,1-2H3
InchiKey: BVQLDIZCFDPYFW-UHFFFAOYSA-N
Formula: C6H12S4
SMILES: CC1CSSSCC(C)S1
Mol. weight [g/mol]: 212.42

Physical Properties

Property code	Value	Unit	Source
gf	151.62	kJ/mol	Joback Method
hf	35.53	kJ/mol	Joback Method
hfus	14.63	kJ/mol	Joback Method
hvap	52.66	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.540		Crippen Method
mcvol	149.940	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1647.00		NIST Webbook
rinpol	1647.00		NIST Webbook
tb	551.42	K	Joback Method
tc	841.91	K	Joback Method
tf	487.28	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.68	J/mol×K	551.42	Joback Method
cpg	331.48	J/mol×K	599.84	Joback Method
cpg	347.97	J/mol×K	648.25	Joback Method
cpg	363.16	J/mol×K	696.67	Joback Method
cpg	377.06	J/mol×K	745.08	Joback Method
cpg	389.69	J/mol×K	793.50	Joback Method
cpg	401.05	J/mol×K	841.91	Joback Method

Sources

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=R225879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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