1,4-dithiacyclohept-5-ene

Inchi: InChI=1S/C5H8S2/c1-2-6-4-5-7-3-1/h1-2H,3-5H2
InchiKey: CXJKJDHACQPAJN-UHFFFAOYSA-N
Formula: C5H8S2
SMILES: C1=CSCCSC1
Mol. weight [g/mol]: 132.25

Physical Properties

Property code	Value	Unit	Source
gf	120.96	kJ/mol	Joback Method
hf	70.27	kJ/mol	Joback Method
hfus	5.91	kJ/mol	Joback Method
hvap	39.55	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.980		Crippen Method
mcvol	98.850	ml/mol	McGowan Method
pc	5022.80	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1107.00		NIST Webbook
tb	437.11	K	Joback Method
tc	693.91	K	Joback Method
tf	321.87	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	168.45	J/mol×K	437.11	Joback Method
cpg	181.59	J/mol×K	479.91	Joback Method
cpg	193.81	J/mol×K	522.71	Joback Method
cpg	205.16	J/mol×K	565.51	Joback Method
cpg	215.66	J/mol×K	608.31	Joback Method
cpg	225.35	J/mol×K	651.11	Joback Method
cpg	234.27	J/mol×K	693.91	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=R82192&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