1,2,3-trithia-5-cycloheptene

Inchi: InChI=1S/C4H6S3/c1-2-4-6-7-5-3-1/h1-2H,3-4H2
InchiKey: MXSCIZUZMRVGGL-UHFFFAOYSA-N
Formula: C4H6S3
SMILES: C1=CCSSSC1
Mol. weight [g/mol]: 150.28

Physical Properties

Property code	Value	Unit	Source
gf	152.40	kJ/mol	Joback Method
hf	136.17	kJ/mol	Joback Method
hfus	6.97	kJ/mol	Joback Method
hvap	43.14	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.586		Crippen Method
mcvol	101.110	ml/mol	McGowan Method
pc	5730.52	kPa	Joback Method
rinpol	1319.00		NIST Webbook
rinpol	1319.00		NIST Webbook
tb	462.06	K	Joback Method
tc	741.84	K	Joback Method
tf	394.05	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	169.03	J/mol×K	462.06	Joback Method
cpg	180.47	J/mol×K	508.69	Joback Method
cpg	190.99	J/mol×K	555.32	Joback Method
cpg	200.63	J/mol×K	601.95	Joback Method
cpg	209.43	J/mol×K	648.58	Joback Method
cpg	217.44	J/mol×K	695.21	Joback Method
cpg	224.71	J/mol×K	741.84	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=R219131&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