Thiacyclononane

Inchi: InChI=1S/C8H16S/c1-2-4-6-8-9-7-5-3-1/h1-8H2
InchiKey: JFPFLSVIMBQNLB-UHFFFAOYSA-N
Formula: C8H16S
SMILES: C1CCCCSCCC1
Mol. weight [g/mol]: 144.28
CAS: 6007-54-1

Physical Properties

Property code	Value	Unit	Source
gf	52.20	kJ/mol	Joback Method
hf	-107.01	kJ/mol	Joback Method
hfus	4.60	kJ/mol	Joback Method
hvap	40.47	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	3.074		Crippen Method
mcvol	129.070	ml/mol	McGowan Method
pc	3547.31	kPa	Joback Method
rinpol	1139.00		NIST Webbook
tb	467.30	K	Joback Method
tc	711.99	K	Joback Method
tf	264.43	K	Joback Method
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.03	J/mol×K	467.30	Joback Method
cpg	281.85	J/mol×K	508.08	Joback Method
cpg	301.45	J/mol×K	548.86	Joback Method
cpg	319.86	J/mol×K	589.65	Joback Method
cpg	337.08	J/mol×K	630.43	Joback Method
cpg	353.14	J/mol×K	671.21	Joback Method
cpg	368.06	J/mol×K	711.99	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35661e+01
Coeff. B	-3.75935e+03
Coeff. C	-7.59500e+01
Temperature range (K), min.	359.06
Temperature range (K), max.	531.37

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R405971&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume