1,2,3-Trithiacyclohexane

Other names: 1,2,3-Trithiane
Inchi: InChI=1S/C3H6S3/c1-2-4-6-5-3-1/h1-3H2
InchiKey: BVOMRRWJQOJMPA-UHFFFAOYSA-N
Formula: C3H6S3
SMILES: C1CSSSC1
Mol. weight [g/mol]: 138.28
CAS: 3325-33-5

Physical Properties

Property code	Value	Unit	Source
gf	126.12	kJ/mol	Joback Method
hf	105.19	kJ/mol	Joback Method
hfus	5.26	kJ/mol	Joback Method
hvap	40.45	kJ/mol	Joback Method
ie	8.36	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
log10ws	-2.60		Crippen Method
logp	2.420		Crippen Method
mcvol	91.320	ml/mol	McGowan Method
pc	6046.69	kPa	Joback Method
rinpol	1216.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1216.00		NIST Webbook
tb	435.75	K	Joback Method
tc	706.04	K	Joback Method
tf	385.54	K	Joback Method
vc	0.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.83	J/mol×K	435.75	Joback Method
cpg	158.30	J/mol×K	480.80	Joback Method

cpg	167.94	J/mol×K	525.85	Joback Method
cpg	176.80	J/mol×K	570.89	Joback Method
cpg	184.93	J/mol×K	615.94	Joback Method
cpg	192.38	J/mol×K	660.99	Joback Method
cpg	199.19	J/mol×K	706.04	Joback Method

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=C3325335&Units=SI

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
ie:	Ionization energy
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