1,3,5-Trithiahexane

Inchi: InChI=1S/C3H8S3/c1-5-3-6-2-4/h4H,2-3H2,1H3
InchiKey: JGXINJXHCVBLHF-UHFFFAOYSA-N
Formula: C3H8S3
SMILES: CSCSCS
Mol. weight [g/mol]: 140.29

Physical Properties

Property code	Value	Unit	Source
gf	70.01	kJ/mol	Joback Method
hf	16.97	kJ/mol	Joback Method
hfus	15.83	kJ/mol	Joback Method
hvap	42.64	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.927		Crippen Method
mcvol	102.180	ml/mol	McGowan Method
pc	5044.23	kPa	Joback Method
rinpol	1146.00		NIST Webbook
tb	468.46	K	Joback Method
tc	716.48	K	Joback Method
tf	228.83	K	Joback Method
vc	0.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.64	J/mol×K	468.46	Joback Method
cpg	185.21	J/mol×K	509.80	Joback Method
cpg	193.37	J/mol×K	551.13	Joback Method
cpg	201.10	J/mol×K	592.47	Joback Method
cpg	208.41	J/mol×K	633.81	Joback Method
cpg	215.28	J/mol×K	675.15	Joback Method
cpg	221.69	J/mol×K	716.48	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=R587187&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
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