1,3,5-Trithiane, 2,4,6-trimethyl, #1

Inchi: InChI=1S/C6H12S3/c1-4-7-5(2)9-6(3)8-4/h4-6H,1-3H3
InchiKey: XQVYLDFSPBXACS-UHFFFAOYSA-N
Formula: C6H12S3
SMILES: CC1SC(C)SC(C)S1
Mol. weight [g/mol]: 180.35

Physical Properties

Property code	Value	Unit	Source
gf	128.25	kJ/mol	Joback Method
hf	-17.75	kJ/mol	Joback Method
hfus	16.24	kJ/mol	Joback Method
hvap	46.20	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.238		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	490.38	K	Joback Method
tc	744.71	K	Joback Method
tf	406.63	K	Joback Method
vc	0.441	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.27	J/mol×K	490.38	Joback Method
cpg	287.41	J/mol×K	532.77	Joback Method
cpg	302.61	J/mol×K	575.16	Joback Method
cpg	316.87	J/mol×K	617.55	Joback Method
cpg	330.21	J/mol×K	659.94	Joback Method
cpg	342.65	J/mol×K	702.32	Joback Method
cpg	354.22	J/mol×K	744.71	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=R44740&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