1,2,4-Trithiolane, 3-methyl-5-(1-methylethyl), #1

Inchi: InChI=1S/C6H12S3/c1-4(2)6-7-5(3)8-9-6/h4-6H,1-3H3
InchiKey: CUDHDMODFNKPPK-UHFFFAOYSA-N
Formula: C6H12S3
SMILES: CC1SSC(C(C)C)S1
Mol. weight [g/mol]: 180.35

Physical Properties

Property code	Value	Unit	Source
gf	145.62	kJ/mol	Joback Method
hf	3.47	kJ/mol	Joback Method
hfus	13.75	kJ/mol	Joback Method
hvap	45.95	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.443		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
rinpol	1279.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1279.00		NIST Webbook
tb	490.34	K	Joback Method
tc	740.91	K	Joback Method
tf	399.39	K	Joback Method
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.89	J/mol×K	490.34	Joback Method
cpg	285.96	J/mol×K	532.10	Joback Method
cpg	300.07	J/mol×K	573.86	Joback Method
cpg	313.24	J/mol×K	615.63	Joback Method
cpg	325.53	J/mol×K	657.39	Joback Method
cpg	336.98	J/mol×K	699.15	Joback Method
cpg	347.62	J/mol×K	740.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62190&Units=SI
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

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