1,2,4-Trithiolane, 3,5-dimethyl, #1

Other names: 3,5-dimethyl-1,2,4-trithiolane, A
Inchi: InChI=1S/C4H8S3/c1-3-5-4(2)7-6-3/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey: HFRUNLRFNNTTPQ-IMJSIDKUSA-N
Formula: C4H8S3
SMILES: CC1SSC(C)S1
Mol. weight [g/mol]: 152.30

Physical Properties

Property code	Value	Unit	Source
gf	131.22	kJ/mol	Joback Method
hf	50.03	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	41.88	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.807		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
rinpol	1161.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1175.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1177.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1593.00		NIST Webbook
ripol	1600.00		NIST Webbook
tb	445.02	K	Joback Method
tc	698.77	K	Joback Method
tf	391.85	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.82	J/mol×K	445.02	Joback Method
cpg	201.68	J/mol×K	487.31	Joback Method
cpg	212.78	J/mol×K	529.60	Joback Method
cpg	223.15	J/mol×K	571.90	Joback Method
cpg	232.82	J/mol×K	614.19	Joback Method
cpg	241.83	J/mol×K	656.48	Joback Method
cpg	250.21	J/mol×K	698.77	Joback Method

Sources

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=R44629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume