3-methyl-1,2,4-trithiolane

Other names: methyl-1,2,4-trithiolane
1,2,4-Trithiolane, 3-methyl
Inchi: InChI=1S/C3H6S3/c1-3-4-2-5-6-3/h3H,2H2,1H3
InchiKey: PWVJWPKTQMWOIH-UHFFFAOYSA-N
Formula: C3H6S3
SMILES: CC1SCSS1
Mol. weight [g/mol]: 138.28

Physical Properties

Property code	Value	Unit	Source
gf	130.51	kJ/mol	Joback Method
hf	91.01	kJ/mol	Joback Method
hfus	8.43	kJ/mol	Joback Method
hvap	39.97	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.418		Crippen Method
mcvol	91.320	ml/mol	McGowan Method
pc	5536.07	kPa	Joback Method
rinpol	1158.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1121.00		NIST Webbook
ripol	1857.00		NIST Webbook
ripol	1857.00		NIST Webbook
tb	426.81	K	Joback Method
tc	685.35	K	Joback Method
tf	384.82	K	Joback Method
vc	0.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.28	J/mol×K	426.81	Joback Method

cpg	161.14	J/mol×K	469.90	Joback Method
cpg	170.27	J/mol×K	512.99	Joback Method
cpg	178.72	J/mol×K	556.08	Joback Method
cpg	186.53	J/mol×K	599.17	Joback Method
cpg	193.74	J/mol×K	642.26	Joback Method
cpg	200.40	J/mol×K	685.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R69180&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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