

1,2,3-Trithiolane

Inchi:	InChI=1S/C2H4S3/c1-2-4-5-3-1/h1-2H2
InchiKey:	LTTGPXZEANXUSL-UHFFFAOYSA-N
Formula:	C2H4S3
SMILES:	C1CSSS1
Mol. weight [g/mol]:	124.25
CAS:	6669-39-2

Physical Properties

Property code	Value	Unit	Source
gf	129.80	kJ/mol	Joback Method
hf	131.99	kJ/mol	Joback Method
hfus	4.77	kJ/mol	Joback Method
hvap	38.05	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	2.030		Crippen Method
mvol	77.230	ml/mol	McGowan Method
pc	6774.04	kPa	Joback Method
rinpol	1068.00		NIST Webbook
tb	408.60	K	Joback Method
tc	671.88	K	Joback Method
tf	377.79	K	Joback Method
vc	0.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.80	J/mol×K	408.60	Joback Method
cpg	122.51	J/mol×K	452.48	Joback Method
cpg	129.53	J/mol×K	496.36	Joback Method
cpg	135.92	J/mol×K	540.24	Joback Method
cpg	141.72	J/mol×K	584.12	Joback Method
cpg	147.00	J/mol×K	628.00	Joback Method
cpg	151.80	J/mol×K	671.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6669392&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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