

1,2,4-Trithiolane, 3,5-diethyl-

Other names:	3,5-Diethyl-1,2,4-trithiolane
Inchi:	InChI=1S/C6H12S3/c1-3-5-7-6(4-2)9-8-5/h5-6H,3-4H2,1-2H3
InchiKey:	WQXXXHMEBYGSBG-UHFFFAOYSA-N
Formula:	C6H12S3
SMILES:	CCC1SSC(CC)S1
Mol. weight [g/mol]:	180.35
CAS:	54644-28-9

Physical Properties

Property code	Value	Unit	Source
gf	148.06	kJ/mol	Joback Method
hf	8.75	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.587		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
ripol	1322.00		NIST Webbook
ripol	1285.80		NIST Webbook
ripol	1292.90		NIST Webbook
ripol	1307.00		NIST Webbook
ripol	1285.80		NIST Webbook
ripol	1359.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1740.00		NIST Webbook
ripol	1744.00		NIST Webbook
ripol	1751.00		NIST Webbook
ripol	1740.00		NIST Webbook
tb	490.78	K	Joback Method
tc	735.25	K	Joback Method
tf	414.39	K	Joback Method
vc	0.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.66	J/mol×K	490.78	Joback Method
cpg	285.28	J/mol×K	531.52	Joback Method
cpg	298.98	J/mol×K	572.27	Joback Method
cpg	311.82	J/mol×K	613.01	Joback Method
cpg	323.82	J/mol×K	653.76	Joback Method
cpg	335.02	J/mol×K	694.50	Joback Method
cpg	345.48	J/mol×K	735.25	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=C54644289&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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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