trans-3,5-Diethyl-1,2,4-trithiolane

Other names: 3,5-Diethyl-1,2,4-trithiolane, (E)-
Inchi: InChI=1S/C6H12S3/c1-3-5-7-6(4-2)9-8-5/h5-6H,3-4H2,1-2H3/t5-,6-/m0/s1
InchiKey: WQXXXHMEBYGSBG-WDSKDSINSA-N
Formula: C6H12S3
SMILES: CCC1SSC(CC)S1
Mol. weight [g/mol]: 180.35
CAS: 38348-26-4

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
rinpol	1333.00		NIST Webbook
rinpol	1333.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1811.00		NIST Webbook
ripol	1797.00		NIST Webbook
tb	490.78	K	Joback Method
tc	735.25	K	Joback Method
tf	414.39	K	Joback Method
vc	0.450	m3/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:	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=C38348264&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