3-ethyl-5-methyl-1,2,4-trithiolane, A

Inchi: InChI=1S/C5H10S3/c1-3-5-6-4(2)7-8-5/h4-5H,3H2,1-2H3
InchiKey: SHLIDHGBMLQTDS-UHFFFAOYSA-N
Formula: C5H10S3
SMILES: CCC1SSC(C)S1
Mol. weight [g/mol]: 166.33

Physical Properties

Property code	Value	Unit	Source
gf	139.64	kJ/mol	Joback Method
hf	29.39	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	44.11	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.197		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
rinpol	1242.00		NIST Webbook
rinpol	1242.00		NIST Webbook
tb	467.90	K	Joback Method
tc	717.05	K	Joback Method
tf	403.12	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.19	J/mol×K	467.90	Joback Method
cpg	242.52	J/mol×K	509.42	Joback Method
cpg	255.01	J/mol×K	550.95	Joback Method
cpg	266.70	J/mol×K	592.47	Joback Method
cpg	277.61	J/mol×K	634.00	Joback Method
cpg	287.79	J/mol×K	675.52	Joback Method
cpg	297.27	J/mol×K	717.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R238667&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume