1,2,4-Trithiolane, 3-ethyl-5-(1-methylethyl), #1

Inchi: InChI=1S/C7H14S3/c1-4-6-8-7(5(2)3)10-9-6/h5-7H,4H2,1-3H3
InchiKey: DLGUSEQUYDDHKA-UHFFFAOYSA-N
Formula: C7H14S3
SMILES: CCC1SSC(C(C)C)S1
Mol. weight [g/mol]: 194.38

Physical Properties

Property code	Value	Unit	Source
gf	154.04	kJ/mol	Joback Method
hf	-17.17	kJ/mol	Joback Method
hfus	16.34	kJ/mol	Joback Method
hvap	48.17	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.833		Crippen Method
mcvol	147.680	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1379.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1377.00		NIST Webbook
tb	513.22	K	Joback Method
tc	758.83	K	Joback Method
tf	410.66	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.40	J/mol×K	513.22	Joback Method
cpg	330.58	J/mol×K	554.15	Joback Method
cpg	345.74	J/mol×K	595.09	Joback Method
cpg	359.92	J/mol×K	636.02	Joback Method
cpg	373.16	J/mol×K	676.96	Joback Method
cpg	385.51	J/mol×K	717.89	Joback Method
cpg	397.01	J/mol×K	758.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R62172&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