6-Ethyl-4,5,7-trithiaoctane

Inchi: InChI=1S/C7H16S3/c1-4-6-9-10-7(5-2)8-3/h7H,4-6H2,1-3H3
InchiKey: RBSQCQCFXKACSX-UHFFFAOYSA-N
Formula: C7H16S3
SMILES: CCCSSC(CC)SC
Mol. weight [g/mol]: 196.40
CAS: 126876-22-0

Physical Properties

Property code	Value	Unit	Source
gf	104.98	kJ/mol	Joback Method
hf	-67.48	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	51.24	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.877		Crippen Method
mcvol	158.540	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1386.20		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1386.20		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1430.70		NIST Webbook
rinpol	1430.70		NIST Webbook
tb	565.46	K	Joback Method
tc	799.82	K	Joback Method
tf	256.85	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.04	J/mol×K	565.46	Joback Method
cpg	361.34	J/mol×K	604.52	Joback Method
cpg	374.85	J/mol×K	643.58	Joback Method

cpg	387.56	J/mol×K	682.64	Joback Method
cpg	399.47	J/mol×K	721.70	Joback Method
cpg	410.57	J/mol×K	760.76	Joback Method
cpg	420.86	J/mol×K	799.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126876220&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