4,5,7,8-Tetrathianonane, 6-ethyl

Inchi:	InChI=1S/C7H16S4/c1-4-6-9-11-7(5-2)10-8-3/h7H,4-6H2,1-3H3
InchiKey:	HBUSMEMTOQGBMV-UHFFFAOYSA-N
Formula:	C7H16S4
SMILES:	CCCSSC(CC)SSC
Mol. weight [g/mol]:	228.46
CAS:	126876-30-0

Physical Properties

Property code	Value	Unit	Source
gf	138.10	kJ/mol	Joback Method
hf	-25.61	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	4.525		Crippen Method
mcvol	174.890	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1685.00		NIST Webbook
rinpol	1685.00		NIST Webbook
rinpol	1646.50		NIST Webbook
rinpol	1646.50		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	634.24	K	Joback Method
tc	887.39	K	Joback Method
tf	291.25	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.86	J/mol×K	634.24	Joback Method
cpg	411.25	J/mol×K	676.43	Joback Method
cpg	424.64	J/mol×K	718.62	Joback Method
cpg	437.03	J/mol×K	760.81	Joback Method

cpg	448.39	J/mol×K	803.01	Joback Method
cpg	458.71	J/mol×K	845.20	Joback Method
cpg	467.97	J/mol×K	887.39	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126876300&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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