4-Ethyl-2,3,5,6-tetrathianonane

Inchi: InChI=1S/C8H18S4/c1-4-6-7-10-12-8(5-2)11-9-3/h8H,4-7H2,1-3H3
InchiKey: LNAMXHMFHVMUIA-UHFFFAOYSA-N
Formula: C8H18S4
SMILES: CCCCSSC(CC)SSC
Mol. weight [g/mol]: 242.49

Physical Properties

Property code	Value	Unit	Source
gf	146.52	kJ/mol	Joback Method
hf	-46.25	kJ/mol	Joback Method
hfus	29.47	kJ/mol	Joback Method
hvap	60.28	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.915		Crippen Method
mcvol	188.980	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
rinpol	1588.50		NIST Webbook
rinpol	1588.50		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	657.12	K	Joback Method
tc	904.57	K	Joback Method
tf	302.52	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.19	J/mol×K	657.12	Joback Method
cpg	461.29	J/mol×K	698.36	Joback Method
cpg	475.34	J/mol×K	739.60	Joback Method
cpg	488.32	J/mol×K	780.84	Joback Method
cpg	500.23	J/mol×K	822.09	Joback Method
cpg	511.04	J/mol×K	863.33	Joback Method
cpg	520.76	J/mol×K	904.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R220710&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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