1,2,4-trithiapentane

Inchi: InChI=1S/C2H6S3/c1-4-2-5-3/h3H,2H2,1H3
InchiKey: WALSYGWNKQSQFW-UHFFFAOYSA-N
Formula: C2H6S3
SMILES: CSCSS
Mol. weight [g/mol]: 126.26

Physical Properties

Property code	Value	Unit	Source
gf	61.59	kJ/mol	Joback Method
hf	37.61	kJ/mol	Joback Method
hfus	13.24	kJ/mol	Joback Method
hvap	40.42	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.885		Crippen Method
mcvol	88.090	ml/mol	McGowan Method
pc	5809.41	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
tb	445.58	K	Joback Method
tc	698.17	K	Joback Method
tf	217.56	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	140.05	J/mol×K	445.58	Joback Method
cpg	146.81	J/mol×K	487.68	Joback Method
cpg	153.28	J/mol×K	529.78	Joback Method
cpg	159.45	J/mol×K	571.87	Joback Method
cpg	165.29	J/mol×K	613.97	Joback Method
cpg	170.80	J/mol×K	656.07	Joback Method
cpg	175.95	J/mol×K	698.17	Joback Method

Sources

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=R226367&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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