1,2,3,5,6-Pentathiepane

Other names: 1,2,3,5,6-Pentathiepane
Lenthionin
Inchi: InChI=1S/C2H4S5/c1-3-4-2-6-7-5-1/h1-2H2
InchiKey: DZKOKXZNCDGVRY-UHFFFAOYSA-N
Formula: C2H4S5
SMILES: C1SSCSSS1
Mol. weight [g/mol]: 188.39

Physical Properties

Property code	Value	Unit	Source
hfus	7.89	kJ/mol	Joback Method
ie	8.59	eV	Cheméo Relay (1.0)
logp	3.326		Crippen Method
mcvol	109.930	ml/mol	McGowan Method
rinpol	1590.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1590.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.21	J/mol×K	512.80	Joback Method
cpg	188.51	J/mol×K	567.08	Joback Method
cpg	196.88	J/mol×K	621.35	Joback Method
cpg	204.37	J/mol×K	675.63	Joback Method
cpg	211.05	J/mol×K	729.91	Joback Method
cpg	216.98	J/mol×K	784.18	Joback Method
cpg	222.22	J/mol×K	838.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C292466&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices