

1,2,4,5-Tetrathiane, 3-methyl-6-pentyl, #2

Inchi:	InChI=1S/C8H16S4/c1-3-4-5-6-8-11-9-7(2)10-12-8/h7-8H,3-6H2,1-2H3
InchiKey:	UFOYXTDAWSLNOL-UHFFFAOYSA-N
Formula:	C8H16S4
SMILES:	CCCCC1SSC(C)SS1
Mol. weight [g/mol]:	240.47

Physical Properties

Property code	Value	Unit	Source
gf	192.66	kJ/mol	Joback Method
hf	6.57	kJ/mol	Joback Method
hfus	24.01	kJ/mol	Joback Method
hvap	56.77	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.015		Crippen Method
mvol	178.120	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1771.00		NIST Webbook
rinpol	1771.00		NIST Webbook
tb	588.64	K	Joback Method
tc	845.01	K	Joback Method
tf	516.86	K	Joback Method
vc	0.600	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.25	J/mol×K	588.64	Joback Method
cpg	423.55	J/mol×K	631.37	Joback Method
cpg	439.68	J/mol×K	674.10	Joback Method
cpg	454.69	J/mol×K	716.83	Joback Method
cpg	468.62	J/mol×K	759.55	Joback Method
cpg	481.52	J/mol×K	802.28	Joback Method
cpg	493.43	J/mol×K	845.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R54456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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