

1,2,4,5-Tetrathiane, 3,6-dimethyl, #1

Inchi: InChI=1S/C4H8S4/c1-3-5-7-4(2)8-6-3/h3-4H,1-2H3/t3-,4-
InchiKey: OLLSVBUNSGNIRV-JPYJGEKTSА-N
Formula: C4H8S4
SMILES: CC1SSC(C)SS1
Mol. weight [g/mol]: 184.37

Physical Properties

Property code	Value	Unit	Source
gf	158.98	kJ/mol	Joback Method
hf	89.13	kJ/mol	Joback Method
hfus	13.65	kJ/mol	Joback Method
hvap	47.87	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.455		Crippen Method
mcvol	121.760	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
rinpol	1343.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1343.00		NIST Webbook
tb	497.12	K	Joback Method
tc	778.61	K	Joback Method
tf	471.78	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.67	J/molxK	497.12	Joback Method
cpg	240.52	J/molxK	544.04	Joback Method
cpg	252.45	J/molxK	590.95	Joback Method
cpg	263.51	J/molxK	637.87	Joback Method
cpg	273.71	J/molxK	684.78	Joback Method
cpg	283.10	J/molxK	731.70	Joback Method
cpg	291.71	J/molxK	778.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R44580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/66-223-1/1-2-4-5-Tetrathiane-3-6-dimethyl-1.pdf>

Generated by Cheméo on 2024-04-17 02:00:02.66729944 +0000 UTC m=+15608451.587876761.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.