

5-Isopropyl-3,3,7,7-tetramethyl-[1,2,4,6]tetrathiepa

Inchi:	InChI=1S/C10H20S4/c1-7(2)8-11-9(3,4)13-14-10(5,6)12-8/h7-8H,1-6H3
InchiKey:	UXSXGLRNACBVGO-UHFFFAOYSA-N
Formula:	C10H20S4
SMILES:	CC(C)C1SC(C)(C)SSC(C)(C)S1
Mol. weight [g/mol]:	268.53

Physical Properties

Property code	Value	Unit	Source
gf	176.27	kJ/mol	Joback Method
hf	-36.01	kJ/mol	Joback Method
hfus	12.04	kJ/mol	Joback Method
hvap	58.39	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.302		Crippen Method
mcvol	206.300	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
tb	634.04	K	Joback Method
tc	916.26	K	Joback Method
tf	564.44	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.18	J/molxK	634.04	Joback Method
cpg	524.51	J/molxK	681.08	Joback Method
cpg	543.80	J/molxK	728.11	Joback Method
cpg	562.46	J/molxK	775.15	Joback Method
cpg	580.91	J/molxK	822.19	Joback Method
cpg	599.57	J/molxK	869.23	Joback Method
cpg	618.83	J/molxK	916.26	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=R495226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/79-000-4/5-Isopropyl-3-3-7-7-tetramethyl-1-2-4-6-tetrathiepane.pdf>

Generated by Cheméo on 2024-05-03 21:21:04.247985324 +0000 UTC m=+17060513.168562645.

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