2,2,4,5-tetramethyl-3-thiahexane

Inchi: InChI=1S/C9H20S/c1-7(2)8(3)10-9(4,5)6/h7-8H,1-6H3
InchiKey: NVNRQXKFNCCXMQ-UHFFFAOYSA-N
Formula: C9H20S
SMILES: CC(C)C(C)SC(C)(C)C
Mol. weight [g/mol]: 160.32

Physical Properties

Property code	Value	Unit	Source
gf	55.98	kJ/mol	Joback Method
hf	-206.53	kJ/mol	Joback Method
hfus	8.74	kJ/mol	Joback Method
hvap	40.37	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.563		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1008.00		NIST Webbook
tb	469.99	K	Joback Method
tc	674.55	K	Joback Method
tf	198.01	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.27	J/mol×K	469.99	Joback Method
cpg	350.38	J/mol×K	504.08	Joback Method
cpg	366.57	J/mol×K	538.18	Joback Method
cpg	381.89	J/mol×K	572.27	Joback Method
cpg	396.35	J/mol×K	606.36	Joback Method
cpg	410.00	J/mol×K	640.46	Joback Method

cpg	422.87	J/mol×K	674.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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