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

Inchi: InChI=1S/C9H20S/c1-7-9(5,6)10-8(2,3)4/h7H2,1-6H3
InchiKey: XZQPSLQNMQTVNC-UHFFFAOYSA-N
Formula: C9H20S
SMILES: CCC(C)(C)SC(C)(C)C
Mol. weight [g/mol]: 160.32

Physical Properties

Property code	Value	Unit	Source
gf	63.70	kJ/mol	Joback Method
hf	-204.72	kJ/mol	Joback Method
hfus	8.37	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.707		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2433.84	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1045.00		NIST Webbook
tb	467.64	K	Joback Method
tc	676.07	K	Joback Method
tf	230.43	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.54	J/mol×K	467.64	Joback Method
cpg	353.20	J/mol×K	502.38	Joback Method
cpg	369.78	J/mol×K	537.12	Joback Method
cpg	385.33	J/mol×K	571.86	Joback Method
cpg	399.90	J/mol×K	606.59	Joback Method
cpg	413.55	J/mol×K	641.33	Joback Method
cpg	426.32	J/mol×K	676.07	Joback Method

Sources

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=R155230&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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