4,4-dimethyl-3-thiahexane

Inchi: InChI=1S/C7H16S/c1-5-7(3,4)8-6-2/h5-6H2,1-4H3
InchiKey: CHNQQTFNKSVKRG-UHFFFAOYSA-N
Formula: C7H16S
SMILES: CCSC(C)(C)CC
Mol. weight [g/mol]: 132.27

Physical Properties

Property code	Value	Unit	Source
gf	44.02	kJ/mol	Joback Method
hf	-154.69	kJ/mol	Joback Method
hfus	10.60	kJ/mol	Joback Method
hvap	36.70	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.928		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	913.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	913.00		NIST Webbook
tb	425.11	K	Joback Method
tc	625.04	K	Joback Method
tf	205.47	K	Joback Method
vc	0.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.74	J/mol×K	425.11	Joback Method
cpg	261.92	J/mol×K	458.43	Joback Method
cpg	275.37	J/mol×K	491.75	Joback Method
cpg	288.12	J/mol×K	525.08	Joback Method
cpg	300.18	J/mol×K	558.40	Joback Method
cpg	311.60	J/mol×K	591.72	Joback Method

cpg	322.39	J/mol×K	625.04	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=R156966&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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