4,5-dimethyl-3-thiahexane

Inchi: InChI=1S/C7H16S/c1-5-8-7(4)6(2)3/h6-7H,5H2,1-4H3
InchiKey: QPTKFJOKFUMHID-UHFFFAOYSA-N
Formula: C7H16S
SMILES: CCSC(C)C(C)C
Mol. weight [g/mol]: 132.27

Physical Properties

Property code	Value	Unit	Source
gf	36.30	kJ/mol	Joback Method
hf	-156.50	kJ/mol	Joback Method
hfus	10.97	kJ/mol	Joback Method
hvap	37.22	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.784		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	928.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	928.00		NIST Webbook
tb	427.46	K	Joback Method
tc	623.67	K	Joback Method
tf	173.05	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.67	J/mol×K	427.46	Joback Method
cpg	259.20	J/mol×K	460.16	Joback Method
cpg	272.18	J/mol×K	492.86	Joback Method
cpg	284.59	J/mol×K	525.56	Joback Method
cpg	296.47	J/mol×K	558.26	Joback Method
cpg	307.81	J/mol×K	590.96	Joback Method

cpg	318.62	J/mol×K	623.67	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=R156971&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