2,4,5-trimethyl-3-thiahexane

Inchi: InChI=1S/C8H18S/c1-6(2)8(5)9-7(3)4/h6-8H,1-5H3
InchiKey: ORHDFBKJWLKEBC-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CC(C)SC(C)C(C)C
Mol. weight [g/mol]: 146.29

Physical Properties

Property code	Value	Unit	Source
gf	42.28	kJ/mol	Joback Method
hf	-182.42	kJ/mol	Joback Method
hfus	10.04	kJ/mol	Joback Method
hvap	39.06	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.172		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
tb	449.90	K	Joback Method
tc	648.57	K	Joback Method
tf	169.32	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.21	J/mol×K	449.90	Joback Method
cpg	302.33	J/mol×K	483.01	Joback Method
cpg	316.79	J/mol×K	516.12	Joback Method
cpg	330.60	J/mol×K	549.24	Joback Method
cpg	343.77	J/mol×K	582.35	Joback Method
cpg	356.32	J/mol×K	615.46	Joback Method

cpg	368.25	J/mol×K	648.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155592&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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