2,2-dimethyl-3-thiaoctane

Inchi: InChI=1S/C9H20S/c1-5-6-7-8-10-9(2,3)4/h5-8H2,1-4H3
InchiKey: UXAUXPUBBOWMBI-UHFFFAOYSA-N
Formula: C9H20S
SMILES: CCCCCSC(C)(C)C
Mol. weight [g/mol]: 160.32

Physical Properties

Property code	Value	Unit	Source
gf	60.86	kJ/mol	Joback Method
hf	-195.97	kJ/mol	Joback Method
hfus	15.78	kJ/mol	Joback Method
hvap	41.15	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.708		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1076.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1073.00		NIST Webbook
tb	470.87	K	Joback Method
tc	666.34	K	Joback Method
tf	228.01	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.03	J/mol×K	470.87	Joback Method
cpg	349.22	J/mol×K	503.45	Joback Method
cpg	364.59	J/mol×K	536.03	Joback Method
cpg	379.17	J/mol×K	568.61	Joback Method
cpg	392.98	J/mol×K	601.18	Joback Method
cpg	406.07	J/mol×K	633.76	Joback Method

cpg	418.46	J/mol×K	666.34	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=R155374&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