2,7-dimethyl-4-thiaoctane

Inchi: InChI=1S/C9H20S/c1-8(2)5-6-10-7-9(3)4/h8-9H,5-7H2,1-4H3
InchiKey: FNXOYWCOEKIXHL-UHFFFAOYSA-N
Formula: C9H20S
SMILES: CC(C)CCSCC(C)C
Mol. weight [g/mol]: 160.32

Physical Properties

Property code	Value	Unit	Source
gf	53.14	kJ/mol	Joback Method
hf	-197.78	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	41.67	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.422		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1096.00		NIST Webbook
tb	473.22	K	Joback Method
tc	665.22	K	Joback Method
tf	195.59	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.70	J/mol×K	473.22	Joback Method
cpg	346.41	J/mol×K	505.22	Joback Method
cpg	361.43	J/mol×K	537.22	Joback Method
cpg	375.80	J/mol×K	569.22	Joback Method
cpg	389.51	J/mol×K	601.22	Joback Method
cpg	402.59	J/mol×K	633.22	Joback Method

cpg	415.05	J/mol×K	665.22	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R155923&Units=SI

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