3,5,5-trimethyl-4-thiaheptane

Inchi: InChI=1S/C9H20S/c1-6-8(3)10-9(4,5)7-2/h8H,6-7H2,1-5H3
InchiKey: CAUBTWNIPVKWEU-UHFFFAOYSA-N
Formula: C9H20S
SMILES: CCC(C)SC(C)(C)CC
Mol. weight [g/mol]: 160.32

Physical Properties

Property code	Value	Unit	Source
gf	58.42	kJ/mol	Joback Method
hf	-201.25	kJ/mol	Joback Method
hfus	12.26	kJ/mol	Joback Method
hvap	40.76	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.707		Crippen Method
mcvol	154.020	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
rinpol	1050.00		NIST Webbook
tb	470.43	K	Joback Method
tc	670.37	K	Joback Method
tf	213.01	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.15	J/mol×K	470.43	Joback Method
cpg	349.79	J/mol×K	503.75	Joback Method
cpg	365.57	J/mol×K	537.08	Joback Method
cpg	380.51	J/mol×K	570.40	Joback Method
cpg	394.65	J/mol×K	603.72	Joback Method
cpg	408.01	J/mol×K	637.04	Joback Method

cpg	420.64	J/mol×K	670.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R156491&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