2,3-dimethyl-4-thiaheptane

Inchi: InChI=1S/C8H18S/c1-5-6-9-8(4)7(2)3/h7-8H,5-6H2,1-4H3
InchiKey: HMVSZFDLCPRNSL-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CCCSC(C)C(C)C
Mol. weight [g/mol]: 146.29

Physical Properties

Property code	Value	Unit	Source
gf	44.72	kJ/mol	Joback Method
hf	-177.14	kJ/mol	Joback Method
hfus	13.56	kJ/mol	Joback Method
hvap	39.44	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	3.174		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1015.00		NIST Webbook
tb	450.34	K	Joback Method
tc	644.50	K	Joback Method
tf	184.32	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.13	J/mol×K	450.34	Joback Method
cpg	301.81	J/mol×K	482.70	Joback Method
cpg	315.88	J/mol×K	515.06	Joback Method
cpg	329.34	J/mol×K	547.42	Joback Method
cpg	342.19	J/mol×K	579.78	Joback Method
cpg	354.46	J/mol×K	612.14	Joback Method
cpg	366.15	J/mol×K	644.50	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=R155512&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