3,3-dimethyl-4-thiaheptane

Inchi: InChI=1S/C8H18S/c1-5-7-9-8(3,4)6-2/h5-7H2,1-4H3
InchiKey: PWRUEOPIIYEEHA-UHFFFAOYSA-N
Formula: C8H18S
SMILES: CCCSC(C)(C)CC
Mol. weight [g/mol]: 146.29

Physical Properties

Property code	Value	Unit	Source
gf	52.44	kJ/mol	Joback Method
hf	-175.33	kJ/mol	Joback Method
hfus	13.19	kJ/mol	Joback Method
hvap	38.92	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.318		Crippen Method
mcvol	139.930	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1000.00		NIST Webbook
tb	447.99	K	Joback Method
tc	645.76	K	Joback Method
tf	216.74	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.36	J/mol×K	447.99	Joback Method
cpg	304.61	J/mol×K	480.95	Joback Method
cpg	319.08	J/mol×K	513.91	Joback Method
cpg	332.81	J/mol×K	546.87	Joback Method
cpg	345.81	J/mol×K	579.83	Joback Method
cpg	358.11	J/mol×K	612.79	Joback Method

cpg	369.75	J/mol×K	645.76	Joback Method

Sources

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=R156451&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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