5,5-dimethyl-4-thia-1-hexyne

Other names: tert.-Butyl propargyl sulfide
Inchi: InChI=1S/C7H12S/c1-5-6-8-7(2,3)4/h1H,6H2,2-4H3
InchiKey: SHONSRZOTAXGMU-UHFFFAOYSA-N
Formula: C7H12S
SMILES: C#CCSC(C)(C)C
Mol. weight [g/mol]: 128.24

Physical Properties

Property code	Value	Unit	Source
gf	267.09	kJ/mol	Joback Method
hf	137.21	kJ/mol	Joback Method
hfus	13.58	kJ/mol	Joback Method
hvap	36.56	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	2.151		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	892.00		NIST Webbook
rinpol	892.00		NIST Webbook
tb	415.23	K	Joback Method
tc	630.66	K	Joback Method
tf	252.44	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.19	J/mol×K	415.23	Joback Method
cpg	232.80	J/mol×K	451.14	Joback Method
cpg	244.64	J/mol×K	487.04	Joback Method
cpg	255.73	J/mol×K	522.95	Joback Method
cpg	266.12	J/mol×K	558.85	Joback Method
cpg	275.84	J/mol×K	594.76	Joback Method
cpg	284.93	J/mol×K	630.66	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=R144077&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