5,5-dimethyl-4-thia-1-heptyne

Other names: 1,1-Dimethylpropyl propargyl sulfide
Inchi: InChI=1S/C8H14S/c1-5-7-9-8(3,4)6-2/h1H,6-7H2,2-4H3
InchiKey: KKLPZDFTGDNLOP-UHFFFAOYSA-N
Formula: C8H14S
SMILES: C#CCSC(C)(C)CC
Mol. weight [g/mol]: 142.26

Physical Properties

Property code	Value	Unit	Source
gf	275.51	kJ/mol	Joback Method
hf	116.57	kJ/mol	Joback Method
hfus	16.17	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.541		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1010.00		NIST Webbook
rinpol	1010.00		NIST Webbook
tb	438.11	K	Joback Method
tc	650.89	K	Joback Method
tf	263.71	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.59	J/mol×K	438.11	Joback Method
cpg	273.43	J/mol×K	473.57	Joback Method
cpg	286.44	J/mol×K	509.04	Joback Method
cpg	298.66	J/mol×K	544.50	Joback Method
cpg	310.12	J/mol×K	579.97	Joback Method
cpg	320.88	J/mol×K	615.43	Joback Method
cpg	330.95	J/mol×K	650.89	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=R144057&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