4-thia-1-hepten-6-yne

Other names: CH«equiv»CCH2SCH2CH=CH2
Inchi: InChI=1S/C6H8S/c1-3-5-7-6-4-2/h1,4H,2,5-6H2
InchiKey: PDTBDBRANSKXPV-UHFFFAOYSA-N
Formula: C6H8S
SMILES: C#CCSCC=C
Mol. weight [g/mol]: 112.19
CAS: 89027-60-1

Physical Properties

Property code	Value	Unit	Source
gf	343.67	kJ/mol	Joback Method
hf	292.03	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	34.95	kJ/mol	Joback Method
log10ws	-1.87		Crippen Method
logp	1.539		Crippen Method
mcvol	98.850	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
rinpol	858.00		NIST Webbook
rinpol	858.00		NIST Webbook
tb	392.26	K	Joback Method
tc	600.09	K	Joback Method
tf	236.99	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.88	J/mol×K	392.26	Joback Method
cpg	175.83	J/mol×K	426.90	Joback Method
cpg	184.31	J/mol×K	461.54	Joback Method
cpg	192.35	J/mol×K	496.17	Joback Method
cpg	199.95	J/mol×K	530.81	Joback Method
cpg	207.15	J/mol×K	565.45	Joback Method

cpg	213.94	J/mol×K	600.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89027601&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

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