2-thia-4-pentyne

Other names: Methyl propargyl sulfide
Inchi: InChI=1S/C4H6S/c1-3-4-5-2/h1H,4H2,2H3
InchiKey: YTXIGMLQHXRSEC-UHFFFAOYSA-N
Formula: C4H6S
SMILES: C#CCSC
Mol. weight [g/mol]: 86.16

Physical Properties

Property code	Value	Unit	Source
gf	238.99	kJ/mol	Joback Method
hf	207.88	kJ/mol	Joback Method
hfus	13.22	kJ/mol	Joback Method
hvap	31.17	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.983		Crippen Method
mcvol	74.970	ml/mol	McGowan Method
pc	4842.69	kPa	Joback Method
rinpol	705.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	705.00		NIST Webbook
tb	349.82	K	Joback Method
tc	555.80	K	Joback Method
tf	216.21	K	Joback Method
vc	0.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.95	J/mol×K	349.82	Joback Method
cpg	121.32	J/mol×K	384.15	Joback Method
cpg	127.41	J/mol×K	418.48	Joback Method
cpg	133.23	J/mol×K	452.81	Joback Method
cpg	138.79	J/mol×K	487.14	Joback Method
cpg	144.08	J/mol×K	521.47	Joback Method

cpg	149.13	J/mol×K	555.80	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=R143950&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