4-thia-1-heptyne

Other names: Propyl propargyl sulfide
Inchi: InChI=1S/C6H10S/c1-3-5-7-6-4-2/h1H,4-6H2,2H3
InchiKey: SQQQEZUUYNQZBQ-UHFFFAOYSA-N
Formula: C6H10S
SMILES: C#CCSCCC
Mol. weight [g/mol]: 114.21

Physical Properties

Property code	Value	Unit	Source
gf	255.83	kJ/mol	Joback Method
hf	166.60	kJ/mol	Joback Method
hfus	18.40	kJ/mol	Joback Method
hvap	35.62	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.763		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	877.00		NIST Webbook
tb	395.58	K	Joback Method
tc	598.73	K	Joback Method
tf	238.75	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.17	J/mol×K	395.58	Joback Method
cpg	190.90	J/mol×K	429.44	Joback Method
cpg	200.18	J/mol×K	463.30	Joback Method
cpg	209.03	J/mol×K	497.15	Joback Method
cpg	217.47	J/mol×K	531.01	Joback Method
cpg	225.50	J/mol×K	564.87	Joback Method

cpg	233.13	J/mol×K	598.73	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=R143990&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