7-methyl-4-thia-1-octyne

Other names: Isopentyll propargyl sulfide
Inchi: InChI=1S/C8H14S/c1-4-6-9-7-5-8(2)3/h1,8H,5-7H2,2-3H3
InchiKey: COFITCLBCKPYPX-UHFFFAOYSA-N
Formula: C8H14S
SMILES: C#CCSCCC(C)C
Mol. weight [g/mol]: 142.26

Physical Properties

Property code	Value	Unit	Source
gf	270.23	kJ/mol	Joback Method
hf	120.04	kJ/mol	Joback Method
hfus	20.06	kJ/mol	Joback Method
hvap	39.69	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.399		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
tb	440.90	K	Joback Method
tc	644.71	K	Joback Method
tf	246.29	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.20	J/mol×K	440.90	Joback Method
cpg	270.03	J/mol×K	474.87	Joback Method
cpg	282.25	J/mol×K	508.84	Joback Method
cpg	293.89	J/mol×K	542.81	Joback Method
cpg	304.94	J/mol×K	576.77	Joback Method
cpg	315.44	J/mol×K	610.74	Joback Method

cpg	325.40	J/mol×K	644.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143896&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