4-thia-1-nonyne

Other names: Pentyl propargyl sulfide
Inchi: InChI=1S/C8H14S/c1-3-5-6-8-9-7-4-2/h2H,3,5-8H2,1H3
InchiKey: OAENEVQWITZHNM-UHFFFAOYSA-N
Formula: C8H14S
SMILES: C#CCSCCCCC
Mol. weight [g/mol]: 142.26

Physical Properties

Property code	Value	Unit	Source
gf	272.67	kJ/mol	Joback Method
hf	125.32	kJ/mol	Joback Method
hfus	23.58	kJ/mol	Joback Method
hvap	40.08	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.543		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1073.00		NIST Webbook
rinpol	1073.00		NIST Webbook
tb	441.34	K	Joback Method
tc	640.42	K	Joback Method
tf	261.29	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.10	J/mol×K	441.34	Joback Method
cpg	269.55	J/mol×K	474.52	Joback Method
cpg	281.42	J/mol×K	507.70	Joback Method
cpg	292.74	J/mol×K	540.88	Joback Method
cpg	303.51	J/mol×K	574.06	Joback Method
cpg	313.76	J/mol×K	607.24	Joback Method
cpg	323.50	J/mol×K	640.42	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=R143821&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