

4-thia-1-nonene

Other names:	Allyl pentyl sulfide
Inchi:	InChI=1S/C8H16S/c1-3-5-6-8-9-7-4-2/h4H,2-3,5-8H2,1H3
InchiKey:	AMSGWDQTSUNZMO-UHFFFAOYSA-N
Formula:	C8H16S
SMILES:	C=CCSCCCCC
Mol. weight [g/mol]:	144.28

Physical Properties

Property code	Value	Unit	Source
gf	137.44	kJ/mol	Joback Method
hf	-41.15	kJ/mol	Joback Method
hfus	19.33	kJ/mol	Joback Method
hvap	39.55	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	3.096		Crippen Method
mcvol	135.630	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1065.00		NIST Webbook
tb	447.90	K	Joback Method
tc	637.40	K	Joback Method
tf	212.56	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.44	J/molxK	447.90	Joback Method
cpg	283.71	J/molxK	479.48	Joback Method
cpg	296.42	J/molxK	511.07	Joback Method
cpg	308.56	J/molxK	542.65	Joback Method
cpg	320.15	J/molxK	574.23	Joback Method
cpg	331.21	J/molxK	605.82	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R143816&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

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