3-Thia-1-octene

Other names: Pentane, 1-ethenylthio
Inchi: InChI=1S/C7H14S/c1-3-5-6-7-8-4-2/h4H,2-3,5-7H2,1H3
InchiKey: HGLZTQUCIJVFCS-UHFFFAOYSA-N
Formula: C7H14S
SMILES: C=CSCCCCC
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	129.02	kJ/mol	Joback Method
hf	-20.51	kJ/mol	Joback Method
hfus	16.74	kJ/mol	Joback Method
hvap	37.32	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.053		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	992.00		NIST Webbook
rinpol	992.00		NIST Webbook
tb	425.02	K	Joback Method
tc	616.35	K	Joback Method
tf	201.29	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.90	J/mol×K	425.02	Joback Method
cpg	242.01	J/mol×K	456.91	Joback Method
cpg	253.60	J/mol×K	488.80	Joback Method
cpg	264.69	J/mol×K	520.69	Joback Method
cpg	275.28	J/mol×K	552.58	Joback Method
cpg	285.38	J/mol×K	584.46	Joback Method
cpg	295.02	J/mol×K	616.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R143801&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