Thiocane

Inchi: InChI=1S/C7H14S/c1-2-4-6-8-7-5-3-1/h1-7H2
InchiKey: AMIGYDGSJCJWSD-UHFFFAOYSA-N
Formula: C7H14S
SMILES: C1CCCSCCC1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	55.88	kJ/mol	Joback Method
hf	-80.21	kJ/mol	Joback Method
hfus	4.11	kJ/mol	Joback Method
hvap	38.07	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.684		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
rinpol	1056.00		NIST Webbook
tb	440.15	K	Joback Method
tc	679.02	K	Joback Method
tf	256.68	K	Joback Method
vc	0.392	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.02	J/mol×K	440.15	Joback Method
cpg	236.50	J/mol×K	479.96	Joback Method
cpg	253.92	J/mol×K	519.77	Joback Method
cpg	270.31	J/mol×K	559.58	Joback Method
cpg	285.68	J/mol×K	599.40	Joback Method
cpg	300.05	J/mol×K	639.21	Joback Method
cpg	313.45	J/mol×K	679.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405986&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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