Thiocyclohex-3-ene, 4-propylidene

Inchi: InChI=1S/C8H12S/c1-2-5-8-6-3-4-7-9-8/h4-5,7H,2-3,6H2,1H3/b8-5+
InchiKey: JWEUCICKWOFJTO-VMPITWQZSA-N
Formula: C8H12S
SMILES: CCC=C1CCC=CS1
Mol. weight [g/mol]: 140.25

Physical Properties

Property code	Value	Unit	Source
gf	163.92	kJ/mol	Joback Method
hf	45.28	kJ/mol	Joback Method
hfus	12.44	kJ/mol	Joback Method
hvap	41.03	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.321		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	1151.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1417.00		NIST Webbook
tb	460.29	K	Joback Method
tc	687.67	K	Joback Method
tf	286.11	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.51	J/mol×K	460.29	Joback Method
cpg	247.15	J/mol×K	498.19	Joback Method
cpg	260.87	J/mol×K	536.08	Joback Method
cpg	273.72	J/mol×K	573.98	Joback Method
cpg	285.74	J/mol×K	611.87	Joback Method
cpg	296.97	J/mol×K	649.77	Joback Method
cpg	307.47	J/mol×K	687.67	Joback Method

Sources

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=R384453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume