

Thiocyclohex-3-ene, 4-methylene

Inchi:	InChI=1S/C6H8S/c1-6-4-2-3-5-7-6/h3,5H,1-2,4H2
InchiKey:	FOQCVEQANNKTBG-UHFFFAOYSA-N
Formula:	C6H8S
SMILES:	C=C1CCC=CS1
Mol. weight [g/mol]:	112.19

Physical Properties

Property code	Value	Unit	Source
gf	154.70	kJ/mol	Joback Method
hf	94.77	kJ/mol	Joback Method
hfus	5.78	kJ/mol	Joback Method
hvap	35.95	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.541		Crippen Method
mcvol	92.290	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpola	970.00		NIST Webbook
ripola	1286.00		NIST Webbook
tb	407.05	K	Joback Method
tc	634.45	K	Joback Method
tf	266.89	K	Joback Method
vc	0.322	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	154.18	J/mol×K	407.05	Joback Method
cpg	165.84	J/mol×K	444.95	Joback Method
cpg	176.79	J/mol×K	482.85	Joback Method
cpg	187.08	J/mol×K	520.75	Joback Method
cpg	196.72	J/mol×K	558.65	Joback Method
cpg	205.74	J/mol×K	596.55	Joback Method
cpg	214.16	J/mol×K	634.45	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R384448&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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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