Thiocyclohex-3-ene, 4-ethylidene

Inchi: InChI=1S/C7H10S/c1-2-7-5-3-4-6-8-7/h2,4,6H,3,5H2,1H3/b7-2+
InchiKey: MJXLEPKLCFQTSJ-FARCUNLSSA-N
Formula: C7H10S
SMILES: CC=C1CCC=CS1
Mol. weight [g/mol]: 126.22

Physical Properties

Property code	Value	Unit	Source
gf	155.50	kJ/mol	Joback Method
hf	65.92	kJ/mol	Joback Method
hfus	9.85	kJ/mol	Joback Method
hvap	38.81	kJ/mol	Joback Method
log10ws	-3.23		Crippen Method
logp	2.931		Crippen Method
mcvol	106.380	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
rinpol	1062.00		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	1373.00		NIST Webbook
ripol	1373.00		NIST Webbook
tb	437.41	K	Joback Method
tc	668.33	K	Joback Method
tf	274.84	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.98	J/mol×K	437.41	Joback Method
cpg	205.39	J/mol×K	475.90	Joback Method
cpg	217.94	J/mol×K	514.38	Joback Method
cpg	229.67	J/mol×K	552.87	Joback Method
cpg	240.63	J/mol×K	591.36	Joback Method
cpg	250.84	J/mol×K	629.85	Joback Method

cpg	260.37	J/mol×K	668.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R384428&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume