Thiocyclohexane, 4-ethylidene

Inchi: InChI=1S/C7H12S/c1-2-7-3-5-8-6-4-7/h2H,3-6H2,1H3
InchiKey: RGDMLMSSMCUUCY-UHFFFAOYSA-N
Formula: C7H12S
SMILES: CC=C1CCSCC1
Mol. weight [g/mol]: 128.24

Physical Properties

Property code	Value	Unit	Source
gf	125.54	kJ/mol	Joback Method
hf	8.14	kJ/mol	Joback Method
hfus	8.63	kJ/mol	Joback Method
hvap	38.51	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.460		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	1047.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1334.00		NIST Webbook
tb	438.25	K	Joback Method
tc	666.68	K	Joback Method
tf	274.08	K	Joback Method
vc	0.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.25	J/mol×K	438.25	Joback Method
cpg	221.09	J/mol×K	476.32	Joback Method
cpg	235.03	J/mol×K	514.39	Joback Method
cpg	248.12	J/mol×K	552.46	Joback Method
cpg	260.39	J/mol×K	590.53	Joback Method
cpg	271.88	J/mol×K	628.61	Joback Method
cpg	282.63	J/mol×K	666.68	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=R384468&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