

Thiocyclohex-3-ene, 4-isopropylidene

Inchi:	InChI=1S/C8H12S/c1-7(2)8-5-3-4-6-9-8/h4,6H,3,5H2,1-2H3
InchiKey:	CWSRYRUWBIEKHS-UHFFFAOYSA-N
Formula:	C8H12S
SMILES:	CC(C)=C1CCC=CS1
Mol. weight [g/mol]:	140.25

Physical Properties

Property code	Value	Unit	Source
gf	155.37	kJ/mol	Joback Method
hf	35.49	kJ/mol	Joback Method
hfus	11.13	kJ/mol	Joback Method
hvap	41.11	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.321		Crippen Method
mcvol	120.470	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook
ripol	1416.00		NIST Webbook
tb	460.17	K	Joback Method
tc	692.29	K	Joback Method
tf	272.15	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.43	J/mol×K	460.17	Joback Method
cpg	247.32	J/mol×K	498.86	Joback Method
cpg	261.26	J/mol×K	537.54	Joback Method
cpg	274.30	J/mol×K	576.23	Joback Method
cpg	286.48	J/mol×K	614.92	Joback Method
cpg	297.84	J/mol×K	653.60	Joback Method
cpg	308.45	J/mol×K	692.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R384433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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