

Thiacyclohexane, 4-methylene

Other names:	Thiacyclohexane, 4-methylene
Inchi:	InChI=1S/C6H10S/c1-6-2-4-7-5-3-6/h1-5H2
InchiKey:	BOJWREQWHOWAEL-UHFFFAOYSA-N
Formula:	C6H10S
SMILES:	C=C1CCSCC1
Mol. weight [g/mol]:	114.21
CAS:	50550-56-6

Physical Properties

Property code	Value	Unit	Source
gf	124.74	kJ/mol	Joback Method
hf	36.99	kJ/mol	Joback Method
hfus	4.56	kJ/mol	Joback Method
hvap	35.66	kJ/mol	Joback Method
ie	9.22	eV	NIST Webbook
log10ws	-1.97		Crippen Method
logp	2.070		Crippen Method
mcvol	96.590	ml/mol	McGowan Method
pc	4200.18	kPa	Joback Method
rinpola	920.00		NIST Webbook
rinpola	920.00		NIST Webbook
ripola	1203.00		NIST Webbook
ripola	1203.00		NIST Webbook
tb	407.89	K	Joback Method
tc	632.80	K	Joback Method
tf	266.13	K	Joback Method
vc	0.336	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.11	J/molxK	407.89	Joback Method
cpg	180.23	J/molxK	445.37	Joback Method
cpg	192.62	J/molxK	482.86	Joback Method

cpg	204.29	J/mol×K	520.34	Joback Method
cpg	215.28	J/mol×K	557.83	Joback Method
cpg	225.61	J/mol×K	595.31	Joback Method
cpg	235.31	J/mol×K	632.80	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=C50550566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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