

Cyclohexane, (methylthio)-

Other names:	Sulfide, cyclohexyl methyl Cyclohexyl methyl sulfide Methylcyclohexylsulfide Methylthiocyclohexane c-C6H11SCH3 Methylsulfanylcyclohexane
Inchi:	InChI=1S/C7H14S/c1-8-7-5-3-2-4-6-7/h7H,2-6H2,1H3
InchiKey:	QQBIOCGHCKNYGP-UHFFFAOYSA-N
Formula:	C7H14S
SMILES:	CSC1CCCCC1
Mol. weight [g/mol]:	130.25
CAS:	7133-37-1

Physical Properties

Property code	Value	Unit	Source
affp	864.50	kJ/mol	NIST Webbook
basg	833.30	kJ/mol	NIST Webbook
gf	65.63	kJ/mol	Joback Method
hf	-91.62	kJ/mol	Joback Method
hfus	9.85	kJ/mol	Joback Method
hvap	38.42	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.682		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	916.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1684.00		NIST Webbook
tb	447.89	K	Joback Method
tc	677.25	K	Joback Method
tf	210.43	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.31	J/mol×K	447.89	Joback Method
cpg	244.48	J/mol×K	486.12	Joback Method
cpg	260.72	J/mol×K	524.34	Joback Method
cpg	276.05	J/mol×K	562.57	Joback Method
cpg	290.48	J/mol×K	600.80	Joback Method
cpg	304.03	J/mol×K	639.03	Joback Method
cpg	316.72	J/mol×K	677.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7133371&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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

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