Cyclohexanemethanethiol

Other names:	Cyclohexylmethanethiol
	Methanethiol, cyclohexyl-
	c-C6H11CH2SH
Inchi:	InChI=1S/C7H14S/c8-6-7-4-2-1-3-5-7/h7-8H,1-6H2
InchiKey:	FWBXAOOHHILPSR-UHFFFAOYSA-N
Formula:	C7H14S
SMILES:	SCC1CCCCC1
Mol. weight [g/mol]:	130.25
CAS:	2550-37-0

Physical Properties

Property code	Value	Unit	Source
affp	813.60	kJ/mol	NIST Webbook
basg	782.40	kJ/mol	NIST Webbook
gf	61.90	kJ/mol	Joback Method
hf	-95.01	kJ/mol	Joback Method
hfus	9.76	kJ/mol	Joback Method
hvap	38.34	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.497		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	1028.00		NIST Webbook
tb	441.97	K	Joback Method
tc	671.52	K	Joback Method
tf	212.49	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.03	J/mol×K	441.97	Joback Method
cpg	242.23	J/mol×K	480.23	Joback Method
cpg	258.44	J/mol×K	518.49	Joback Method

cpg	273.70	J/mol×K	556.75	Joback Method
cpg	288.04	J/mol×K	595.00	Joback Method
cpg	301.49	J/mol×K	633.26	Joback Method
cpg	314.07	J/mol×K	671.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2550370&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume