Cyclohexanethiol, 2-methyl-, cis-

Inchi: InChI=1S/C7H14S/c1-6-4-2-3-5-7(6)8/h6-8H,2-5H2,1H3/t6-,7+/m0/s1
InchiKey: ICOZZYFCTGILJV-NKWVEPMBSA-N
Formula: C7H14S
SMILES: CC1CCCCC1S
Mol. weight [g/mol]: 130.25
CAS: 22425-07-6

Physical Properties

Property code	Value	Unit	Source
gf	54.19	kJ/mol	Joback Method
hf	-115.35	kJ/mol	Joback Method
hfus	10.83	kJ/mol	Joback Method
hvap	38.03	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.495		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
rinpol	988.00		NIST Webbook
tb	434.00 ± 4.00	K	NIST Webbook
tc	666.53	K	Joback Method
tf	208.25	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.46	J/mol×K	437.30	Joback Method
cpg	243.00	J/mol×K	475.50	Joback Method
cpg	259.60	J/mol×K	513.71	Joback Method
cpg	275.28	J/mol×K	551.91	Joback Method
cpg	290.07	J/mol×K	590.12	Joback Method
cpg	303.98	J/mol×K	628.32	Joback Method
cpg	317.03	J/mol×K	666.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22425076&Units=SI

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