1-Methylcyclohexane-1-thiol

Inchi: InChI=1S/C7H14S/c1-7(8)5-3-2-4-6-7/h8H,2-6H2,1H3
InchiKey: OPVQCLPKQYQDFG-UHFFFAOYSA-N
Formula: C7H14S
SMILES: CC1(S)CCCCC1
Mol. weight [g/mol]: 130.25

Physical Properties

Property code	Value	Unit	Source
gf	56.41	kJ/mol	Joback Method
hf	-79.77	kJ/mol	Joback Method
hfus	3.46	kJ/mol	Joback Method
hvap	37.19	kJ/mol	Joback Method
log10ws	-2.83		Crippen Method
logp	2.639		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	968.00		NIST Webbook
tb	442.21	K	Joback Method
tc	682.63	K	Joback Method
tf	236.39	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.86	J/mol×K	442.21	Joback Method
cpg	243.46	J/mol×K	482.28	Joback Method
cpg	259.67	J/mol×K	522.35	Joback Method
cpg	274.62	J/mol×K	562.42	Joback Method
cpg	288.47	J/mol×K	602.49	Joback Method
cpg	301.37	J/mol×K	642.56	Joback Method
cpg	313.46	J/mol×K	682.63	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=R524146&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