Hexane-4-thiol, 1-methoxy

Inchi: InChI=1S/C7H16OS/c1-3-7(9)5-4-6-8-2/h7,9H,3-6H2,1-2H3
InchiKey: ONKCGFJYPKAYEH-UHFFFAOYSA-N
Formula: C7H16OS
SMILES: CCC(S)CCCOC
Mol. weight [g/mol]: 148.27

Physical Properties

Property code	Value	Unit	Source
gf	-69.99	kJ/mol	Joback Method
hf	-286.83	kJ/mol	Joback Method
hfus	15.59	kJ/mol	Joback Method
hvap	39.94	kJ/mol	Joback Method
log10ws	-2.02		Crippen Method
logp	2.121		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
rinpol	1062.00		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1406.00		NIST Webbook
tb	444.40	K	Joback Method
tc	635.25	K	Joback Method
tf	212.34	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.46	J/mol×K	444.40	Joback Method
cpg	280.28	J/mol×K	476.21	Joback Method
cpg	292.62	J/mol×K	508.02	Joback Method
cpg	304.47	J/mol×K	539.82	Joback Method
cpg	315.85	J/mol×K	571.63	Joback Method
cpg	326.76	J/mol×K	603.44	Joback Method

cpg	337.20	J/mol×K	635.25	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=R402338&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume