(+/-)-1-Methoxy-4-methylpentane-3-thiol

Inchi: InChI=1S/C7H16OS/c1-6(2)7(9)4-5-8-3/h6-7,9H,4-5H2,1-3H3
InchiKey: MXDSGTTVQNVYGY-UHFFFAOYSA-N
Formula: C7H16OS
SMILES: COCCC(S)C(C)C
Mol. weight [g/mol]: 148.27

Physical Properties

Property code	Value	Unit	Source
gf	-72.43	kJ/mol	Joback Method
hf	-292.11	kJ/mol	Joback Method
hfus	12.07	kJ/mol	Joback Method
hvap	39.55	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.977		Crippen Method
mcvol	131.710	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1029.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	443.96	K	Joback Method
tc	639.24	K	Joback Method
tf	197.34	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	267.55	J/mol×K	443.96	Joback Method
cpg	280.76	J/mol×K	476.51	Joback Method
cpg	293.45	J/mol×K	509.05	Joback Method
cpg	305.63	J/mol×K	541.60	Joback Method
cpg	317.30	J/mol×K	574.14	Joback Method
cpg	328.47	J/mol×K	606.69	Joback Method
cpg	339.14	J/mol×K	639.24	Joback Method

Sources

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=R504291&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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