Hexanethioic acid, S-methyl ester

Other names: Methanethiol caproate
Methylthiohexanoate
S-methyl hexanethioate
Inchi: InChI=1S/C7H14OS/c1-3-4-5-6-7(8)9-2/h3-6H2,1-2H3
InchiKey: AKGAHYLJHAOPKQ-UHFFFAOYSA-N
Formula: C7H14OS
SMILES: CCCCCC(=O)SC
Mol. weight [g/mol]: 146.25
CAS: 2432-77-1

Physical Properties

Property code	Value	Unit	Source
gf	-87.74	kJ/mol	Joback Method
hf	-258.52	kJ/mol	Joback Method
hfus	19.62	kJ/mol	Joback Method
hvap	44.74	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.456		Crippen Method
mcvol	127.410	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	1074.00		NIST Webbook
rinpol	1073.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1073.00		NIST Webbook
ripol	1412.00		NIST Webbook
tb	482.21	K	Joback Method
tc	680.42	K	Joback Method
tf	252.98	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.46	J/mol×K	482.21	Joback Method

cpg	276.49	J/mol×K	515.24	Joback Method
cpg	288.00	J/mol×K	548.28	Joback Method
cpg	298.98	J/mol×K	581.31	Joback Method
cpg	309.45	J/mol×K	614.35	Joback Method
cpg	319.41	J/mol×K	647.38	Joback Method
cpg	328.87	J/mol×K	680.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2432771&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

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