Octanethioic acid, S-methyl ester

Other names: S-Methyl thiooctanoate
Inchi: InChI=1S/C9H18OS/c1-3-4-5-6-7-8-9(10)11-2/h3-8H2,1-2H3
InchiKey: UKPKZMMTLNIPKR-UHFFFAOYSA-N
Formula: C9H18OS
SMILES: CCCCCCCC(=O)SC
Mol. weight [g/mol]: 174.30
CAS: 2432-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-70.90	kJ/mol	Joback Method
hf	-299.80	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.236		Crippen Method
mcvol	155.590	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1293.00		NIST Webbook
tb	527.97	K	Joback Method
tc	721.15	K	Joback Method
tf	275.52	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.66	J/mol×K	527.97	Joback Method
cpg	366.67	J/mol×K	560.17	Joback Method
cpg	380.04	J/mol×K	592.36	Joback Method
cpg	392.79	J/mol×K	624.56	Joback Method
cpg	404.92	J/mol×K	656.75	Joback Method
cpg	416.45	J/mol×K	688.95	Joback Method
cpg	427.39	J/mol×K	721.15	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=C2432839&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