Ethanethioic acid, S-phenyl ester

Other names:	Acetic acid, thio-, S-phenyl ester
	Phenyl thioacetate
	S-Phenyl thioacetate
	Phenyl thiolacetate
	Thiophenyl acetate
	Thioacetic acid S-phenyl ester
Inchi:	InChI=1S/C8H8OS/c1-7(9)10-8-5-3-2-4-6-8/h2-6H,1H3
InchiKey:	WBISVCLTLBMTDS-UHFFFAOYSA-N
Formula:	C8H8OS
SMILES:	CC(=O)Sc1ccccc1
Mol. weight [g/mol]:	152.21
CAS:	934-87-2

Physical Properties

Property code	Value	Unit	Source
gf	33.09	kJ/mol	Joback Method
hf	-42.63	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	2.325		Crippen Method
mcvol	117.740	ml/mol	McGowan Method
pc	4031.24	kPa	Joback Method
tb	531.77	K	Joback Method
tc	776.43	K	Joback Method
tf	290.67	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.47	J/mol×K	531.77	Joback Method
cpg	249.47	J/mol×K	572.55	Joback Method
cpg	260.61	J/mol×K	613.32	Joback Method

cpg	270.92	J/mol×K	654.10	Joback Method
cpg	280.43	J/mol×K	694.88	Joback Method
cpg	289.16	J/mol×K	735.65	Joback Method
cpg	297.16	J/mol×K	776.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.70	K	0.80	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C934872&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume