(Phenylthio)acetic acid methyl ester

Other names:	Methyl (phenylthio)acetate
	Acetic acid, (phenylthio)-, methyl ester
	Methyl phenylsulfenylacetate
Inchi:	InChI=1S/C9H10O2S/c1-11-9(10)7-12-8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	MUNSXQQODXYRKI-UHFFFAOYSA-N
Formula:	C9H10O2S
SMILES:	COC(=O)CSc1ccccc1
Mol. weight [g/mol]:	182.24
CAS:	17277-58-6

Physical Properties

Property code	Value	Unit	Source
gf	-63.49	kJ/mol	Joback Method
hf	-195.49	kJ/mol	Joback Method
hfus	20.02	kJ/mol	Joback Method
hvap	53.88	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.952		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
tb	577.07	K	Joback Method
tc	813.29	K	Joback Method
tf	324.17	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.29	J/mol×K	577.07	Joback Method
cpg	317.08	J/mol×K	616.44	Joback Method
cpg	329.02	J/mol×K	655.81	Joback Method
cpg	340.13	J/mol×K	695.18	Joback Method
cpg	350.42	J/mol×K	734.55	Joback Method
cpg	359.90	J/mol×K	773.92	Joback Method

cpg	368.59	J/mol×K	813.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17277586&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume