Phenylthioacetic acid, 4-methoxyphenyl ester

Inchi: InChI=1S/C15H14O3S/c1-17-12-7-9-13(10-8-12)18-15(16)11-19-14-5-3-2-4-6-14/h2-10H
InchiKey: AEJAHBFFBIJZEE-UHFFFAOYSA-N
Formula: C15H14O3S
SMILES: COc1ccc(OC(=O)CSc2ccccc2)cc1
Mol. weight [g/mol]: 274.33

Physical Properties

Property code	Value	Unit	Source
gf	-15.19	kJ/mol	Joback Method
hf	-226.49	kJ/mol	Joback Method
hfus	30.40	kJ/mol	Joback Method
hvap	72.58	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.393		Crippen Method
mcvol	204.350	ml/mol	McGowan Method
pc	2589.85	kPa	Joback Method
rinpol	2234.00		NIST Webbook
tb	768.43	K	Joback Method
tc	1018.25	K	Joback Method
tf	452.96	K	Joback Method
vc	0.755	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.94	J/mol×K	768.43	Joback Method
cpg	558.09	J/mol×K	810.07	Joback Method
cpg	570.88	J/mol×K	851.70	Joback Method
cpg	582.34	J/mol×K	893.34	Joback Method
cpg	592.47	J/mol×K	934.98	Joback Method
cpg	601.31	J/mol×K	976.62	Joback Method
cpg	608.87	J/mol×K	1018.25	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=U307776&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume