(Phenylthio)acetic acid, (4-methoxyphenyl)methyl ester

Inchi: InChI=1S/C16H16O3S/c1-18-14-9-7-13(8-10-14)11-19-16(17)12-20-15-5-3-2-4-6-15/h2-1

InchiKey: YFBVYQWUOYICDE-UHFFFAOYSA-N

Formula: C16H16O3S

SMILES: COc1ccc(COC(=O)CSc2ccccc2)cc1

Mol. weight [g/mol]: 288.36

Physical Properties

Property code	Value	Unit	Source
gf	-6.77	kJ/mol	Joback Method
hf	-247.13	kJ/mol	Joback Method
hfus	32.99	kJ/mol	Joback Method
hvap	74.81	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.531		Crippen Method
mcvol	218.440	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	2308.00		NIST Webbook
tb	791.31	K	Joback Method
tc	1036.12	K	Joback Method
tf	464.23	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.98	J/mol×K	791.31	Joback Method
cpg	612.36	J/mol×K	832.11	Joback Method
cpg	625.36	J/mol×K	872.91	Joback Method
cpg	637.01	J/mol×K	913.72	Joback Method
cpg	647.33	J/mol×K	954.52	Joback Method
cpg	656.35	J/mol×K	995.32	Joback Method
cpg	664.09	J/mol×K	1036.12	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=U308339&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