Benzeneacetic acid, 2,5-dimethoxy-4-propylthio, methyl ester

Inchi: InChI=1S/C14H20O4S/c1-5-6-19-13-9-11(16-2)10(7-12(13)17-3)8-14(15)18-4/h7,9H,5-6,

InchiKey: INXGDHLDEGRBHC-UHFFFAOYSA-N

Formula: C14H20O4S

SMILES: CCCSc1cc(OC)c(CC(=O)OC)cc1OC

Mol. weight [g/mol]: 284.37

Physical Properties

Property code	Value	Unit	Source
gf	-260.28	kJ/mol	Joback Method
hf	-597.54	kJ/mol	Joback Method
hfus	34.18	kJ/mol	Joback Method
hvap	71.81	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.921		Crippen Method
mcvol	219.890	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	1950.00		NIST Webbook
tb	751.25	K	Joback Method
tc	964.89	K	Joback Method
tf	462.54	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.10	J/mol×K	751.25	Joback Method
cpg	618.85	J/mol×K	786.86	Joback Method
cpg	632.59	J/mol×K	822.46	Joback Method
cpg	645.29	J/mol×K	858.07	Joback Method
cpg	656.92	J/mol×K	893.68	Joback Method
cpg	667.46	J/mol×K	929.28	Joback Method
cpg	676.89	J/mol×K	964.89	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=R418516&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