Benzeneethanol, 2,5-dimethoxy-4-propylthio, acetate

Inchi: InChI=1S/C15H22O4S/c1-5-8-20-15-10-13(17-3)12(9-14(15)18-4)6-7-19-11(2)16/h9-10H

InchiKey: UKRIFYCTPFVBTE-UHFFFAOYSA-N

Formula: C15H22O4S

SMILES: CCCSc1cc(OC)c(CCOC(C)=O)cc1OC

Mol. weight [g/mol]: 298.40

Physical Properties

Property code	Value	Unit	Source
gf	-251.86	kJ/mol	Joback Method
hf	-618.18	kJ/mol	Joback Method
hfus	36.77	kJ/mol	Joback Method
hvap	74.04	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.312		Crippen Method
mcvol	233.980	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2080.00		NIST Webbook
tb	774.13	K	Joback Method
tc	985.38	K	Joback Method
tf	473.81	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	659.25	J/mol×K	774.13	Joback Method
cpg	674.30	J/mol×K	809.34	Joback Method
cpg	688.28	J/mol×K	844.55	Joback Method
cpg	701.17	J/mol×K	879.75	Joback Method
cpg	712.94	J/mol×K	914.96	Joback Method
cpg	723.58	J/mol×K	950.17	Joback Method
cpg	733.06	J/mol×K	985.38	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=R418521&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