(Phenylthio)acetic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C13H12O2S/c1-2-3-7-10-15-13(14)11-16-12-8-5-4-6-9-12/h1,3-9H,10-11H2
InchiKey: ILXWVEBJXABYAM-UHFFFAOYSA-N
Formula: C13H12O2S
SMILES: C#CC=CCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 232.30

Physical Properties

Property code	Value	Unit	Source
gf	273.48	kJ/mol	Joback Method
hf	131.07	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	62.60	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.511		Crippen Method
mcvol	181.160	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tb	662.87	K	Joback Method
tc	906.27	K	Joback Method
tf	411.14	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.31	J/mol×K	662.87	Joback Method
cpg	445.97	J/mol×K	703.44	Joback Method
cpg	458.57	J/mol×K	744.00	Joback Method
cpg	470.17	J/mol×K	784.57	Joback Method
cpg	480.83	J/mol×K	825.14	Joback Method
cpg	490.60	J/mol×K	865.70	Joback Method
cpg	499.54	J/mol×K	906.27	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=U299422&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