(Phenylthio)acetic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C14H16O2S/c1-3-8-12(4-2)16-14(15)11-17-13-9-6-5-7-10-13/h5-7,9-10,12H,4,
InchiKey: MILNALODDHZVED-UHFFFAOYSA-N
Formula: C14H16O2S
SMILES: CC#CC(CC)OC(=O)CSc1ccccc1
Mol. weight [g/mol]: 248.34

Physical Properties

Property code	Value	Unit	Source
gf	178.97	kJ/mol	Joback Method
hf	-31.67	kJ/mol	Joback Method
hfus	32.57	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.124		Crippen Method
mcvol	199.550	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	700.03	K	Joback Method
tc	943.85	K	Joback Method
tf	471.62	K	Joback Method
vc	0.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.89	J/mol×K	700.03	Joback Method
cpg	523.54	J/mol×K	740.67	Joback Method
cpg	538.00	J/mol×K	781.30	Joback Method
cpg	551.30	J/mol×K	821.94	Joback Method
cpg	563.47	J/mol×K	862.58	Joback Method
cpg	574.53	J/mol×K	903.21	Joback Method
cpg	584.52	J/mol×K	943.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299423&Units=SI
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

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