(Phenylthio)acetic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C12H12O2S/c1-3-10(2)14-12(13)9-15-11-7-5-4-6-8-11/h1,4-8,10H,9H2,2H3
InchiKey: PBTHHOIYSNWFQQ-UHFFFAOYSA-N
Formula: C12H12O2S
SMILES: C#CC(C)OC(=O)CSc1ccccc1
Mol. weight [g/mol]: 220.29

Physical Properties

Property code	Value	Unit	Source
gf	182.40	kJ/mol	Joback Method
hf	29.21	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	60.03	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.344		Crippen Method
mcvol	171.370	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1582.00		NIST Webbook
tb	635.39	K	Joback Method
tc	878.92	K	Joback Method
tf	389.95	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.68	J/mol×K	635.39	Joback Method
cpg	419.73	J/mol×K	675.98	Joback Method
cpg	432.72	J/mol×K	716.57	Joback Method
cpg	444.69	J/mol×K	757.15	Joback Method
cpg	455.68	J/mol×K	797.74	Joback Method
cpg	465.71	J/mol×K	838.33	Joback Method
cpg	474.82	J/mol×K	878.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299420&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