(Phenylthio)acetic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C18H22O2S/c1-14(2)10-11-16(12-15(3)4)20-18(19)13-21-17-8-6-5-7-9-17/h5-9

InchiKey: MFSURPYVUFOBQQ-UHFFFAOYSA-N

Formula: C18H22O2S

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)CSc1ccccc1

Mol. weight [g/mol]: 302.43

Physical Properties

Property code	Value	Unit	Source
gf	289.50	kJ/mol	Joback Method
hf	-3.87	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.316		Crippen Method
mcvol	251.610	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2068.00		NIST Webbook
tb	787.67	K	Joback Method
tc	1025.42	K	Joback Method
tf	485.98	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.08	J/mol×K	787.67	Joback Method
cpg	716.78	J/mol×K	827.30	Joback Method
cpg	732.15	J/mol×K	866.92	Joback Method
cpg	746.25	J/mol×K	906.55	Joback Method
cpg	759.12	J/mol×K	946.17	Joback Method
cpg	770.81	J/mol×K	985.80	Joback Method
cpg	781.37	J/mol×K	1025.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299425&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