(Phenylthio)acetic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H22O2S/c1-4-5-9-15(12-14(2)3)19-17(18)13-20-16-10-7-6-8-11-16/h6-8,10

InchiKey: YBZPKHKRWRYUIK-UHFFFAOYSA-N

Formula: C17H22O2S

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

Mol. weight [g/mol]: 290.42

Physical Properties

Property code	Value	Unit	Source
gf	201.79	kJ/mol	Joback Method
hf	-98.87	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.150		Crippen Method
mcvol	241.820	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook
tb	768.23	K	Joback Method
tc	1002.50	K	Joback Method
tf	490.43	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.31	J/mol×K	768.23	Joback Method
cpg	687.15	J/mol×K	807.27	Joback Method
cpg	702.69	J/mol×K	846.32	Joback Method
cpg	716.96	J/mol×K	885.36	Joback Method
cpg	730.01	J/mol×K	924.41	Joback Method
cpg	741.86	J/mol×K	963.45	Joback Method
cpg	752.56	J/mol×K	1002.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299424&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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