(Phenylthio)acetic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C19H24O2S/c1-5-9-16(4)18(13-12-15(2)3)21-19(20)14-22-17-10-7-6-8-11-17/h

InchiKey: AQPWGSQNSKAZGU-UHFFFAOYSA-N

Formula: C19H24O2S

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

Mol. weight [g/mol]: 316.46

Physical Properties

Property code	Value	Unit	Source
gf	297.92	kJ/mol	Joback Method
hf	-24.51	kJ/mol	Joback Method
hfus	39.41	kJ/mol	Joback Method
hvap	76.92	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	4.706		Crippen Method
mcvol	265.700	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2150.00		NIST Webbook
tb	810.55	K	Joback Method
tc	1044.36	K	Joback Method
tf	497.25	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.58	J/mol×K	810.55	Joback Method
cpg	773.39	J/mol×K	849.52	Joback Method
cpg	788.88	J/mol×K	888.49	Joback Method
cpg	803.09	J/mol×K	927.45	Joback Method
cpg	816.07	J/mol×K	966.42	Joback Method
cpg	827.88	J/mol×K	1005.39	Joback Method
cpg	838.56	J/mol×K	1044.36	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299426&Units=SI

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