(Phenylthio)acetic acid, dodec-9-ynyl ester

Inchi: InChI=1S/C20H28O2S/c1-2-3-4-5-6-7-8-9-10-14-17-22-20(21)18-23-19-15-12-11-13-16-1
InchiKey: BMBCZUYMRAIGMT-UHFFFAOYSA-N
Formula: C20H28O2S
SMILES: CCC#CCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 332.50

Physical Properties

Property code	Value	Unit	Source
gf	231.93	kJ/mol	Joback Method
hf	-150.23	kJ/mol	Joback Method
hfus	51.64	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.466		Crippen Method
mcvol	284.090	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2548.00		NIST Webbook
tb	837.75	K	Joback Method
tc	1056.07	K	Joback Method
tf	554.24	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.40	J/mol×K	837.75	Joback Method
cpg	857.10	J/mol×K	874.14	Joback Method
cpg	872.57	J/mol×K	910.52	Joback Method
cpg	886.84	J/mol×K	946.91	Joback Method
cpg	899.96	J/mol×K	983.29	Joback Method
cpg	911.97	J/mol×K	1019.68	Joback Method
cpg	922.90	J/mol×K	1056.07	Joback Method

Sources

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=U299960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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