(Phenylthio)acetic acid, undec-10-enyl ester

Inchi: InChI=1S/C19H28O2S/c1-2-3-4-5-6-7-8-9-13-16-21-19(20)17-22-18-14-11-10-12-15-18/h
InchiKey: HRLFUSLYOOAIFI-UHFFFAOYSA-N
Formula: C19H28O2S
SMILES: C=CCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 320.49

Physical Properties

Property code	Value	Unit	Source
gf	108.55	kJ/mol	Joback Method
hf	-276.46	kJ/mol	Joback Method
hfus	44.64	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.629		Crippen Method
mcvol	274.300	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook
tb	802.55	K	Joback Method
tc	1009.36	K	Joback Method
tf	435.11	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.95	J/mol×K	802.55	Joback Method
cpg	822.59	J/mol×K	837.02	Joback Method
cpg	838.09	J/mol×K	871.49	Joback Method
cpg	852.51	J/mol×K	905.95	Joback Method
cpg	865.88	J/mol×K	940.42	Joback Method
cpg	878.24	J/mol×K	974.89	Joback Method
cpg	889.63	J/mol×K	1009.36	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=U299848&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