(Phenylthio)acetic acid, undecyl ester

Inchi: InChI=1S/C19H30O2S/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: WDKLUCFGPFOJMA-UHFFFAOYSA-N
Formula: C19H30O2S
SMILES: CCCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 322.50

Physical Properties

Property code	Value	Unit	Source
gf	20.71	kJ/mol	Joback Method
hf	-401.89	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.853		Crippen Method
mcvol	278.600	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	2409.00		NIST Webbook
rinpol	2409.00		NIST Webbook
tb	805.87	K	Joback Method
tc	1010.34	K	Joback Method
tf	436.87	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.49	J/mol×K	805.87	Joback Method
cpg	849.60	J/mol×K	839.95	Joback Method
cpg	865.56	J/mol×K	874.03	Joback Method
cpg	880.40	J/mol×K	908.10	Joback Method
cpg	894.16	J/mol×K	942.18	Joback Method
cpg	906.88	J/mol×K	976.26	Joback Method
cpg	918.59	J/mol×K	1010.34	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=U299959&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