(Phenylthio)acetic acid, nonyl ester

Inchi: InChI=1S/C17H26O2S/c1-2-3-4-5-6-7-11-14-19-17(18)15-20-16-12-9-8-10-13-16/h8-10,1
InchiKey: UVWUXWMBLPVCSX-UHFFFAOYSA-N
Formula: C17H26O2S
SMILES: CCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 294.45

Physical Properties

Property code	Value	Unit	Source
gf	3.87	kJ/mol	Joback Method
hf	-360.61	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	71.69	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.073		Crippen Method
mcvol	250.420	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2190.00		NIST Webbook
tb	760.11	K	Joback Method
tc	967.40	K	Joback Method
tf	414.33	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.45	J/mol×K	760.11	Joback Method
cpg	734.20	J/mol×K	794.66	Joback Method
cpg	749.84	J/mol×K	829.21	Joback Method
cpg	764.41	J/mol×K	863.76	Joback Method
cpg	777.93	J/mol×K	898.30	Joback Method
cpg	790.44	J/mol×K	932.85	Joback Method
cpg	801.96	J/mol×K	967.40	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=U299956&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