(Phenylthio)acetic acid, 5-tetradecyl ester

Inchi: InChI=1S/C22H36O2S/c1-3-5-7-8-9-10-12-16-20(15-6-4-2)24-22(23)19-25-21-17-13-11-
InchiKey: BJFWQIFXNVNCED-UHFFFAOYSA-N
Formula: C22H36O2S
SMILES: CCCCCCCCCC(CCCC)OC(=O)CSc1ccccc1
Mol. weight [g/mol]: 364.58

Physical Properties

Property code	Value	Unit	Source
gf	43.53	kJ/mol	Joback Method
hf	-469.09	kJ/mol	Joback Method
hfus	50.17	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	7.021		Crippen Method
mcvol	320.870	ml/mol	McGowan Method
pc	1166.43	kPa	Joback Method
tb	874.07	K	Joback Method
tc	1080.61	K	Joback Method
tf	455.68	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1011.83	J/mol×K	874.07	Joback Method
cpg	1029.51	J/mol×K	908.49	Joback Method
cpg	1045.92	J/mol×K	942.92	Joback Method
cpg	1061.10	J/mol×K	977.34	Joback Method
cpg	1075.11	J/mol×K	1011.76	Joback Method
cpg	1087.98	J/mol×K	1046.19	Joback Method
cpg	1099.76	J/mol×K	1080.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299910&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume