(Phenylthio)acetic acid, 3-pentadecyl ester

Inchi: InChI=1S/C23H38O2S/c1-3-5-6-7-8-9-10-11-12-14-17-21(4-2)25-23(24)20-26-22-18-15-1
InchiKey: NURUGLLITAETTA-UHFFFAOYSA-N
Formula: C23H38O2S
SMILES: CCCCCCCCCCCCC(CC)OC(=O)CSc1ccccc1
Mol. weight [g/mol]: 378.61

Physical Properties

Property code	Value	Unit	Source
gf	51.95	kJ/mol	Joback Method
hf	-489.73	kJ/mol	Joback Method
hfus	52.76	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-7.89		Crippen Method
logp	7.411		Crippen Method
mcvol	334.960	ml/mol	McGowan Method
pc	1093.54	kPa	Joback Method
tb	896.95	K	Joback Method
tc	1104.78	K	Joback Method
tf	466.95	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.85	J/mol×K	896.95	Joback Method
cpg	1090.66	J/mol×K	931.59	Joback Method
cpg	1107.16	J/mol×K	966.23	Joback Method
cpg	1122.41	J/mol×K	1000.87	Joback Method
cpg	1136.45	J/mol×K	1035.51	Joback Method
cpg	1149.33	J/mol×K	1070.14	Joback Method
cpg	1161.10	J/mol×K	1104.78	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=U299911&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume