(Phenylthio)acetic acid, 5-tridecyl ester

Inchi: InChI=1S/C21H34O2S/c1-3-5-7-8-9-11-15-19(14-6-4-2)23-21(22)18-24-20-16-12-10-13-1
InchiKey: IVJYMRIBCBWQBO-UHFFFAOYSA-N
Formula: C21H34O2S
SMILES: CCCCCCCCC(CCCC)OC(=O)CSc1ccccc1
Mol. weight [g/mol]: 350.56

Physical Properties

Property code	Value	Unit	Source
gf	35.11	kJ/mol	Joback Method
hf	-448.45	kJ/mol	Joback Method
hfus	47.58	kJ/mol	Joback Method
hvap	80.20	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.631		Crippen Method
mcvol	306.780	ml/mol	McGowan Method
pc	1246.85	kPa	Joback Method
tb	851.19	K	Joback Method
tc	1057.19	K	Joback Method
tf	444.41	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	951.48	J/mol×K	851.19	Joback Method
cpg	969.04	J/mol×K	885.52	Joback Method
cpg	985.35	J/mol×K	919.86	Joback Method
cpg	1000.48	J/mol×K	954.19	Joback Method
cpg	1014.44	J/mol×K	988.52	Joback Method
cpg	1027.30	J/mol×K	1022.86	Joback Method
cpg	1039.08	J/mol×K	1057.19	Joback Method

Sources

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=U299907&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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