(Phenylthio)acetic acid, 4-hexadecyl ester

Inchi: InChI=1S/C24H40O2S/c1-3-5-6-7-8-9-10-11-12-14-18-22(17-4-2)26-24(25)21-27-23-19-1
InchiKey: WIZLMQDSYOEMEG-UHFFFAOYSA-N
Formula: C24H40O2S
SMILES: CCCCCCCCCCCCC(CCC)OC(=O)CSc1ccccc1
Mol. weight [g/mol]: 392.64

Physical Properties

Property code	Value	Unit	Source
gf	60.37	kJ/mol	Joback Method
hf	-510.37	kJ/mol	Joback Method
hfus	55.35	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.802		Crippen Method
mcvol	349.050	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpol	2768.00		NIST Webbook
rinpol	2768.00		NIST Webbook
tb	919.83	K	Joback Method
tc	1129.77	K	Joback Method
tf	478.22	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.47	J/mol×K	919.83	Joback Method
cpg	1152.43	J/mol×K	954.82	Joback Method
cpg	1169.04	J/mol×K	989.81	Joback Method
cpg	1184.36	J/mol×K	1024.80	Joback Method
cpg	1198.44	J/mol×K	1059.79	Joback Method
cpg	1211.32	J/mol×K	1094.78	Joback Method
cpg	1223.08	J/mol×K	1129.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299961&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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