(Phenylthio)acetic acid, hexadecyl ester

Inchi: InChI=1S/C24H40O2S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-26-24(25)22-27-23-19-
InchiKey: XUTDABKADWXICQ-UHFFFAOYSA-N
Formula: C24H40O2S
SMILES: CCCCCCCCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 392.64

Physical Properties

Property code	Value	Unit	Source
gf	62.81	kJ/mol	Joback Method
hf	-505.09	kJ/mol	Joback Method
hfus	58.87	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.803		Crippen Method
mcvol	349.050	ml/mol	McGowan Method
pc	1022.04	kPa	Joback Method
rinpol	2934.00		NIST Webbook
rinpol	2934.00		NIST Webbook
tb	920.27	K	Joback Method
tc	1129.35	K	Joback Method
tf	493.22	K	Joback Method
vc	1.349	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.04	J/mol×K	920.27	Joback Method
cpg	1151.96	J/mol×K	955.12	Joback Method
cpg	1168.55	J/mol×K	989.96	Joback Method
cpg	1183.88	J/mol×K	1024.81	Joback Method
cpg	1197.98	J/mol×K	1059.65	Joback Method
cpg	1210.92	J/mol×K	1094.50	Joback Method
cpg	1222.74	J/mol×K	1129.35	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=U299853&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume