(Phenylthio)acetic acid, pentadecyl ester

Inchi: InChI=1S/C23H38O2S/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-25-23(24)21-26-22-18-15-1
InchiKey: SCFJLJQQNNDISM-UHFFFAOYSA-N
Formula: C23H38O2S
SMILES: CCCCCCCCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 378.61

Physical Properties

Property code	Value	Unit	Source
gf	54.39	kJ/mol	Joback Method
hf	-484.45	kJ/mol	Joback Method
hfus	56.28	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	7.413		Crippen Method
mcvol	334.960	ml/mol	McGowan Method
pc	1087.78	kPa	Joback Method
rinpol	2815.00		NIST Webbook
tb	897.39	K	Joback Method
tc	1104.00	K	Joback Method
tf	481.95	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1072.39	J/mol×K	897.39	Joback Method
cpg	1090.12	J/mol×K	931.83	Joback Method
cpg	1106.58	J/mol×K	966.26	Joback Method
cpg	1121.80	J/mol×K	1000.70	Joback Method
cpg	1135.84	J/mol×K	1035.13	Joback Method
cpg	1148.75	J/mol×K	1069.57	Joback Method
cpg	1160.57	J/mol×K	1104.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299852&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume