(Phenylthio)acetic acid, heptadecyl ester

Inchi: InChI=1S/C25H42O2S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-27-25(26)23-28-24-2
InchiKey: OPUIWWIJLMCXDQ-UHFFFAOYSA-N
Formula: C25H42O2S
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 406.67

Physical Properties

Property code	Value	Unit	Source
gf	71.23	kJ/mol	Joback Method
hf	-525.73	kJ/mol	Joback Method
hfus	61.46	kJ/mol	Joback Method
hvap	89.49	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.193		Crippen Method
mcvol	363.140	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	3101.00		NIST Webbook
rinpol	3101.00		NIST Webbook
tb	943.15	K	Joback Method
tc	1155.57	K	Joback Method
tf	504.49	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1196.24	J/mol×K	943.15	Joback Method
cpg	1214.38	J/mol×K	978.55	Joback Method
cpg	1231.13	J/mol×K	1013.96	Joback Method
cpg	1246.57	J/mol×K	1049.36	Joback Method
cpg	1260.74	J/mol×K	1084.76	Joback Method
cpg	1273.70	J/mol×K	1120.17	Joback Method
cpg	1285.53	J/mol×K	1155.57	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=U299962&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