(Phenylthio) acetic acid, octadecyl ester

Inchi: InChI=1S/C26H44O2S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-23-28-26(27)24-29-2
InchiKey: LLEQKQGEZSVVFL-UHFFFAOYSA-N
Formula: C26H44O2S
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 420.69

Physical Properties

Property code	Value	Unit	Source
gf	79.65	kJ/mol	Joback Method
hf	-546.37	kJ/mol	Joback Method
hfus	64.05	kJ/mol	Joback Method
hvap	91.72	kJ/mol	Joback Method
log10ws	-9.03		Crippen Method
logp	8.583		Crippen Method
mcvol	377.230	ml/mol	McGowan Method
pc	907.24	kPa	Joback Method
rinpol	3233.00		NIST Webbook
rinpol	3233.00		NIST Webbook
tb	966.03	K	Joback Method
tc	1182.75	K	Joback Method
tf	515.76	K	Joback Method
vc	1.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1258.95	J/mol×K	966.03	Joback Method
cpg	1277.33	J/mol×K	1002.15	Joback Method
cpg	1294.27	J/mol×K	1038.27	Joback Method
cpg	1309.83	J/mol×K	1074.39	Joback Method
cpg	1324.08	J/mol×K	1110.51	Joback Method
cpg	1337.08	J/mol×K	1146.63	Joback Method
cpg	1348.90	J/mol×K	1182.75	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=U299854&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