(Phenylthio)acetic acid, decyl ester

Inchi: InChI=1S/C18H28O2S/c1-2-3-4-5-6-7-8-12-15-20-18(19)16-21-17-13-10-9-11-14-17/h9-1
InchiKey: XDUXLYYUKXSPMR-UHFFFAOYSA-N
Formula: C18H28O2S
SMILES: CCCCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 308.48

Physical Properties

Property code	Value	Unit	Source
gf	12.29	kJ/mol	Joback Method
hf	-381.25	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	5.463		Crippen Method
mcvol	264.510	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2297.00		NIST Webbook
rinpol	2297.00		NIST Webbook
tb	782.99	K	Joback Method
tc	988.58	K	Joback Method
tf	425.60	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.50	J/mol×K	782.99	Joback Method
cpg	791.44	J/mol×K	817.26	Joback Method
cpg	807.26	J/mol×K	851.52	Joback Method
cpg	821.98	J/mol×K	885.79	Joback Method
cpg	835.63	J/mol×K	920.05	Joback Method
cpg	848.26	J/mol×K	954.32	Joback Method
cpg	859.89	J/mol×K	988.58	Joback Method

Sources

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=U299847&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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