(Phenylthio)acetic acid, hexyl ester

Inchi: InChI=1S/C14H20O2S/c1-2-3-4-8-11-16-14(15)12-17-13-9-6-5-7-10-13/h5-7,9-10H,2-4,8
InchiKey: RVHAPFYENYJEOV-UHFFFAOYSA-N
Formula: C14H20O2S
SMILES: CCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 252.37

Physical Properties

Property code	Value	Unit	Source
gf	-21.39	kJ/mol	Joback Method
hf	-298.69	kJ/mol	Joback Method
hfus	32.97	kJ/mol	Joback Method
hvap	65.01	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.902		Crippen Method
mcvol	208.150	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1843.00		NIST Webbook
tb	691.47	K	Joback Method
tc	906.83	K	Joback Method
tf	380.52	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.64	J/mol×K	691.47	Joback Method
cpg	568.55	J/mol×K	727.36	Joback Method
cpg	583.42	J/mol×K	763.26	Joback Method
cpg	597.27	J/mol×K	799.15	Joback Method
cpg	610.13	J/mol×K	835.04	Joback Method
cpg	622.02	J/mol×K	870.93	Joback Method
cpg	632.97	J/mol×K	906.83	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=U299844&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