(Phenylthio)acetic acid, cyclohexyl ester

Inchi: InChI=1S/C14H18O2S/c15-14(16-12-7-3-1-4-8-12)11-17-13-9-5-2-6-10-13/h2,5-6,9-10,1
InchiKey: SIRIXPOWYMQWOJ-UHFFFAOYSA-N
Formula: C14H18O2S
SMILES: O=C(CSc1ccccc1)OC1CCCCC1
Mol. weight [g/mol]: 250.36

Physical Properties

Property code	Value	Unit	Source
gf	3.06	kJ/mol	Joback Method
hf	-244.37	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.655		Crippen Method
mcvol	197.290	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1939.00		NIST Webbook
tb	711.02	K	Joback Method
tc	962.47	K	Joback Method
tf	387.90	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.14	J/mol×K	711.02	Joback Method
cpg	563.74	J/mol×K	752.93	Joback Method
cpg	580.73	J/mol×K	794.84	Joback Method
cpg	596.17	J/mol×K	836.75	Joback Method
cpg	610.09	J/mol×K	878.66	Joback Method
cpg	622.54	J/mol×K	920.57	Joback Method
cpg	633.57	J/mol×K	962.47	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=U308354&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