(Phenylthio)acetic acid, 1-cyclopentylethyl ester

Inchi: InChI=1S/C15H20O2S/c1-12(13-7-5-6-8-13)17-15(16)11-18-14-9-3-2-4-10-14/h2-4,9-10,

InchiKey: FSWCJCGGAHDFEM-UHFFFAOYSA-N

Formula: C15H20O2S

SMILES: CC(OC(=O)CSc1ccccc1)C1CCCC1

Mol. weight [g/mol]: 264.38

Physical Properties

Property code	Value	Unit	Source
gf	21.14	kJ/mol	Joback Method
hf	-264.13	kJ/mol	Joback Method
hfus	25.98	kJ/mol	Joback Method
hvap	67.10	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.901		Crippen Method
mcvol	211.380	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	729.19	K	Joback Method
tc	972.54	K	Joback Method
tf	387.69	K	Joback Method
vc	0.780	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.23	J/mol×K	729.19	Joback Method
cpg	615.56	J/mol×K	769.75	Joback Method
cpg	632.38	J/mol×K	810.31	Joback Method
cpg	647.74	J/mol×K	850.87	Joback Method
cpg	661.70	J/mol×K	891.42	Joback Method
cpg	674.32	J/mol×K	931.98	Joback Method
cpg	685.65	J/mol×K	972.54	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=U308355&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