(Phenylthio)acetic acid, cyclopentyl ester

Inchi: InChI=1S/C13H16O2S/c14-13(15-11-6-4-5-7-11)10-16-12-8-2-1-3-9-12/h1-3,8-9,11H,4-7
InchiKey: ZTXZIMSUBNBDCR-UHFFFAOYSA-N
Formula: C13H16O2S
SMILES: O=C(CSc1ccccc1)OC1CCCC1
Mol. weight [g/mol]: 236.33

Physical Properties

Property code	Value	Unit	Source
gf	6.74	kJ/mol	Joback Method
hf	-217.57	kJ/mol	Joback Method
hfus	24.32	kJ/mol	Joback Method
hvap	63.04	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.264		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	683.87	K	Joback Method
tc	932.91	K	Joback Method
tf	380.15	K	Joback Method
vc	0.674	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.33	J/mol×K	683.87	Joback Method
cpg	506.85	J/mol×K	725.38	Joback Method
cpg	522.93	J/mol×K	766.88	Joback Method
cpg	537.62	J/mol×K	808.39	Joback Method
cpg	550.98	J/mol×K	849.89	Joback Method
cpg	563.04	J/mol×K	891.40	Joback Method
cpg	573.87	J/mol×K	932.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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