Phenylthioacetic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C14H11ClO2S/c15-11-6-8-12(9-7-11)17-14(16)10-18-13-4-2-1-3-5-13/h1-9H,1
InchiKey: RODRARCUWYZGJA-UHFFFAOYSA-N
Formula: C14H11ClO2S
SMILES: O=C(CSc1ccccc1)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 278.75

Physical Properties

Property code	Value	Unit	Source
gf	69.46	kJ/mol	Joback Method
hf	-89.37	kJ/mol	Joback Method
hfus	30.82	kJ/mol	Joback Method
hvap	72.33	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.038		Crippen Method
mcvol	196.630	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	760.56	K	Joback Method
tc	1022.16	K	Joback Method
tf	449.38	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.67	J/mol×K	760.56	Joback Method
cpg	501.54	J/mol×K	804.16	Joback Method
cpg	513.10	J/mol×K	847.76	Joback Method
cpg	523.40	J/mol×K	891.36	Joback Method
cpg	532.48	J/mol×K	934.96	Joback Method
cpg	540.41	J/mol×K	978.56	Joback Method
cpg	547.22	J/mol×K	1022.16	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307774&Units=SI

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