Phenylthioacetic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C14H10Cl2O2S/c15-12-7-6-10(8-13(12)16)18-14(17)9-19-11-4-2-1-3-5-11/h1-8

InchiKey: BDFGZZWWXMDBOI-UHFFFAOYSA-N

Formula: C14H10Cl2O2S

SMILES: O=C(CSc1ccccc1)Oc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 313.20

Physical Properties

Property code	Value	Unit	Source
gf	47.90	kJ/mol	Joback Method
hf	-116.58	kJ/mol	Joback Method
hfus	34.63	kJ/mol	Joback Method
hvap	77.38	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.691		Crippen Method
mcvol	208.870	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	802.97	K	Joback Method
tc	1066.72	K	Joback Method
tf	491.82	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.92	J/mol×K	802.97	Joback Method
cpg	519.24	J/mol×K	846.93	Joback Method
cpg	529.31	J/mol×K	890.89	Joback Method
cpg	538.15	J/mol×K	934.85	Joback Method
cpg	545.83	J/mol×K	978.80	Joback Method
cpg	552.37	J/mol×K	1022.76	Joback Method
cpg	557.82	J/mol×K	1066.72	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=U307778&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