Phenylthioacetic acid, 3-methylphenyl ester

Inchi: InChI=1S/C15H14O2S/c1-12-6-5-7-13(10-12)17-15(16)11-18-14-8-3-2-4-9-14/h2-10H,11
InchiKey: FOTMXUDCRYSQAE-UHFFFAOYSA-N
Formula: C15H14O2S
SMILES: Cc1cccc(OC(=O)CSc2ccccc2)c1
Mol. weight [g/mol]: 258.33

Physical Properties

Property code	Value	Unit	Source
gf	89.81	kJ/mol	Joback Method
hf	-94.27	kJ/mol	Joback Method
hfus	29.22	kJ/mol	Joback Method
hvap	70.17	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.693		Crippen Method
mcvol	198.480	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	746.01	K	Joback Method
tc	1000.02	K	Joback Method
tf	430.73	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.37	J/mol×K	746.01	Joback Method
cpg	533.06	J/mol×K	788.34	Joback Method
cpg	546.41	J/mol×K	830.68	Joback Method
cpg	558.45	J/mol×K	873.01	Joback Method
cpg	569.23	J/mol×K	915.35	Joback Method
cpg	578.80	J/mol×K	957.68	Joback Method
cpg	587.21	J/mol×K	1000.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307773&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