Phenylthioacetic acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C16H16O2S/c1-12-8-13(2)10-14(9-12)18-16(17)11-19-15-6-4-3-5-7-15/h3-10H

InchiKey: NZVQTZHEGBMVOZ-UHFFFAOYSA-N

Formula: C16H16O2S

SMILES: Cc1cc(C)cc(OC(=O)CSc2ccccc2)c1

Mol. weight [g/mol]: 272.36

Physical Properties

Property code	Value	Unit	Source
gf	88.60	kJ/mol	Joback Method
hf	-126.38	kJ/mol	Joback Method
hfus	31.42	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.001		Crippen Method
mcvol	212.570	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	2150.00		NIST Webbook
tb	773.87	K	Joback Method
tc	1023.18	K	Joback Method
tf	454.52	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.62	J/mol×K	773.87	Joback Method
cpg	585.46	J/mol×K	815.42	Joback Method
cpg	598.97	J/mol×K	856.97	Joback Method
cpg	611.17	J/mol×K	898.52	Joback Method
cpg	622.12	J/mol×K	940.08	Joback Method
cpg	631.84	J/mol×K	981.63	Joback Method
cpg	640.38	J/mol×K	1023.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307775&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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