(Phenylthio)acetic acid, 3-phenylpropyl ester

Inchi: InChI=1S/C17H18O2S/c18-17(14-20-16-11-5-2-6-12-16)19-13-7-10-15-8-3-1-4-9-15/h1-6
InchiKey: FURQRGUDFUEJKS-UHFFFAOYSA-N
Formula: C17H18O2S
SMILES: O=C(CSc1ccccc1)OCCCc1ccccc1
Mol. weight [g/mol]: 286.39

Physical Properties

Property code	Value	Unit	Source
gf	116.28	kJ/mol	Joback Method
hf	-124.08	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	73.96	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.955		Crippen Method
mcvol	226.660	ml/mol	McGowan Method
pc	2214.53	kPa	Joback Method
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
tb	786.79	K	Joback Method
tc	1029.71	K	Joback Method
tf	440.75	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.59	J/mol×K	786.79	Joback Method
cpg	642.89	J/mol×K	827.28	Joback Method
cpg	656.81	J/mol×K	867.76	Joback Method
cpg	669.42	J/mol×K	908.25	Joback Method
cpg	680.77	J/mol×K	948.74	Joback Method
cpg	690.92	J/mol×K	989.22	Joback Method
cpg	699.94	J/mol×K	1029.71	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=U308358&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