(Phenylthio)acetic acid, phenylmethyl ester

Inchi: InChI=1S/C15H14O2S/c16-15(12-18-14-9-5-2-6-10-14)17-11-13-7-3-1-4-8-13/h1-10H,11
InchiKey: HFNGWLVGBRAPAH-UHFFFAOYSA-N
Formula: C15H14O2S
SMILES: O=C(CSc1ccccc1)OCc1ccccc1
Mol. weight [g/mol]: 258.33

Physical Properties

Property code	Value	Unit	Source
gf	99.44	kJ/mol	Joback Method
hf	-82.80	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	69.51	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.522		Crippen Method
mcvol	198.480	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	2050.00		NIST Webbook
tb	741.03	K	Joback Method
tc	994.27	K	Joback Method
tf	418.21	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	519.65	J/mol×K	741.03	Joback Method
cpg	534.49	J/mol×K	783.24	Joback Method
cpg	547.95	J/mol×K	825.44	Joback Method
cpg	560.10	J/mol×K	867.65	Joback Method
cpg	570.98	J/mol×K	909.85	Joback Method
cpg	580.65	J/mol×K	952.06	Joback Method
cpg	589.18	J/mol×K	994.27	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=U308338&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