(Phenylthio)acetic acid, 2-phenylethyl ester

Inchi: InChI=1S/C16H16O2S/c17-16(13-19-15-9-5-2-6-10-15)18-12-11-14-7-3-1-4-8-14/h1-10H
InchiKey: MTUKAPTVYMHMMJ-UHFFFAOYSA-N
Formula: C16H16O2S
SMILES: O=C(CSc1ccccc1)OCCc1ccccc1
Mol. weight [g/mol]: 272.36

Physical Properties

Property code	Value	Unit	Source
gf	107.86	kJ/mol	Joback Method
hf	-103.44	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	71.74	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.565		Crippen Method
mcvol	212.570	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	2163.00		NIST Webbook
rinpol	2163.00		NIST Webbook
tb	763.91	K	Joback Method
tc	1011.73	K	Joback Method
tf	429.48	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.09	J/mol×K	763.91	Joback Method
cpg	588.20	J/mol×K	805.21	Joback Method
cpg	601.92	J/mol×K	846.52	Joback Method
cpg	614.33	J/mol×K	887.82	Joback Method
cpg	625.48	J/mol×K	929.12	Joback Method
cpg	635.43	J/mol×K	970.43	Joback Method
cpg	644.23	J/mol×K	1011.73	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=U308357&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