(Phenylthio)acetic acid, pentyl ester

Inchi: InChI=1S/C13H18O2S/c1-2-3-7-10-15-13(14)11-16-12-8-5-4-6-9-12/h4-6,8-9H,2-3,7,10-1
InchiKey: CGTJOPWTGGHEGM-UHFFFAOYSA-N
Formula: C13H18O2S
SMILES: CCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 238.35

Physical Properties

Property code	Value	Unit	Source
gf	-29.81	kJ/mol	Joback Method
hf	-278.05	kJ/mol	Joback Method
hfus	30.38	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.512		Crippen Method
mcvol	194.060	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	668.59	K	Joback Method
tc	887.49	K	Joback Method
tf	369.25	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.10	J/mol×K	668.59	Joback Method
cpg	515.60	J/mol×K	705.07	Joback Method
cpg	530.07	J/mol×K	741.56	Joback Method
cpg	543.56	J/mol×K	778.04	Joback Method
cpg	556.08	J/mol×K	814.52	Joback Method
cpg	567.66	J/mol×K	851.00	Joback Method
cpg	578.31	J/mol×K	887.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299843&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