(Phenylthio)acetic acid, butyl ester

Inchi: InChI=1S/C12H16O2S/c1-2-3-9-14-12(13)10-15-11-7-5-4-6-8-11/h4-8H,2-3,9-10H2,1H3
InchiKey: MPGIAEVWEVYNKM-UHFFFAOYSA-N
Formula: C12H16O2S
SMILES: CCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 224.32

Physical Properties

Property code	Value	Unit	Source
gf	-38.23	kJ/mol	Joback Method
hf	-257.41	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.122		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1672.00		NIST Webbook
tb	645.71	K	Joback Method
tc	868.50	K	Joback Method
tf	357.98	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.90	J/mol×K	645.71	Joback Method
cpg	463.89	J/mol×K	682.84	Joback Method
cpg	477.90	J/mol×K	719.97	Joback Method
cpg	490.95	J/mol×K	757.11	Joback Method
cpg	503.05	J/mol×K	794.24	Joback Method
cpg	514.24	J/mol×K	831.37	Joback Method
cpg	524.52	J/mol×K	868.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299842&Units=SI

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