(Phenylthio)acetic acid, propyl ester

Inchi: InChI=1S/C11H14O2S/c1-2-8-13-11(12)9-14-10-6-4-3-5-7-10/h3-7H,2,8-9H2,1H3
InchiKey: PGNCCKPNZYBMHV-UHFFFAOYSA-N
Formula: C11H14O2S
SMILES: CCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 210.29

Physical Properties

Property code	Value	Unit	Source
gf	-46.65	kJ/mol	Joback Method
hf	-236.77	kJ/mol	Joback Method
hfus	25.20	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.732		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1567.00		NIST Webbook
rinpol	1567.00		NIST Webbook
tb	622.83	K	Joback Method
tc	849.84	K	Joback Method
tf	346.71	K	Joback Method
vc	0.622	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.14	J/mol×K	622.83	Joback Method
cpg	413.52	J/mol×K	660.66	Joback Method
cpg	426.96	J/mol×K	698.50	Joback Method
cpg	439.47	J/mol×K	736.33	Joback Method
cpg	451.07	J/mol×K	774.17	Joback Method
cpg	461.78	J/mol×K	812.00	Joback Method
cpg	471.62	J/mol×K	849.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308337&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