(Phenylthio)acetic acid, 3-methylbut-2-enyl ester

Inchi: InChI=1S/C13H16O2S/c1-11(2)8-9-15-13(14)10-16-12-6-4-3-5-7-12/h3-8H,9-10H2,1-2H3

InchiKey: OYZUVMGOIHHXCB-UHFFFAOYSA-N

Formula: C13H16O2S

SMILES: CC(C)=CCOC(=O)CSc1ccccc1

Mol. weight [g/mol]: 236.33

Physical Properties

Property code	Value	Unit	Source
gf	41.86	kJ/mol	Joback Method
hf	-170.62	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	62.82	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.288		Crippen Method
mcvol	189.760	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
tb	672.63	K	Joback Method
tc	904.12	K	Joback Method
tf	350.21	K	Joback Method
vc	0.715	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.41	J/mol×K	672.63	Joback Method
cpg	492.54	J/mol×K	711.21	Joback Method
cpg	506.60	J/mol×K	749.79	Joback Method
cpg	519.63	J/mol×K	788.38	Joback Method
cpg	531.68	J/mol×K	826.96	Joback Method
cpg	542.78	J/mol×K	865.54	Joback Method
cpg	552.99	J/mol×K	904.12	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=U299421&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