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

Inchi: InChI=1S/C11H11ClO2S/c12-7-4-8-14-11(13)9-15-10-5-2-1-3-6-10/h1-7H,8-9H2/b7-4+

InchiKey: RUHVHMBFVMISGJ-QPJJXVBHSA-N

Formula: C11H11ClO2S

SMILES: O=C(CSc1ccccc1)OCC=CCl

Mol. weight [g/mol]: 242.72

Physical Properties

Property code	Value	Unit	Source
gf	21.64	kJ/mol	Joback Method
hf	-135.29	kJ/mol	Joback Method
hfus	29.60	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.074		Crippen Method
mcvol	173.820	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1765.00		NIST Webbook
tb	664.42	K	Joback Method
tc	904.24	K	Joback Method
tf	371.55	K	Joback Method
vc	0.650	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.94	J/mol×K	664.42	Joback Method
cpg	414.55	J/mol×K	704.39	Joback Method
cpg	426.17	J/mol×K	744.36	Joback Method
cpg	436.86	J/mol×K	784.33	Joback Method
cpg	446.65	J/mol×K	824.30	Joback Method
cpg	455.58	J/mol×K	864.27	Joback Method
cpg	463.70	J/mol×K	904.24	Joback Method

Sources

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=U299429&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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