(Phenylthio)acetic acid, heptyl ester

Inchi: InChI=1S/C15H22O2S/c1-2-3-4-5-9-12-17-15(16)13-18-14-10-7-6-8-11-14/h6-8,10-11H,2
InchiKey: CGQZJXYQJQDCGP-UHFFFAOYSA-N
Formula: C15H22O2S
SMILES: CCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 266.40

Physical Properties

Property code	Value	Unit	Source
gf	-12.97	kJ/mol	Joback Method
hf	-319.33	kJ/mol	Joback Method
hfus	35.56	kJ/mol	Joback Method
hvap	67.23	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.292		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1902.00		NIST Webbook
tb	714.35	K	Joback Method
tc	926.56	K	Joback Method
tf	391.79	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	606.44	J/mol×K	714.35	Joback Method
cpg	622.68	J/mol×K	749.72	Joback Method
cpg	637.86	J/mol×K	785.09	Joback Method
cpg	652.01	J/mol×K	820.46	Joback Method
cpg	665.14	J/mol×K	855.83	Joback Method
cpg	677.29	J/mol×K	891.19	Joback Method
cpg	688.48	J/mol×K	926.56	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=U299845&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