(Phenylthio)acetic acid, octyl ester

Inchi: InChI=1S/C16H24O2S/c1-2-3-4-5-6-10-13-18-16(17)14-19-15-11-8-7-9-12-15/h7-9,11-12
InchiKey: QGVZNJTVKALZLR-UHFFFAOYSA-N
Formula: C16H24O2S
SMILES: CCCCCCCCOC(=O)CSc1ccccc1
Mol. weight [g/mol]: 280.43

Physical Properties

Property code	Value	Unit	Source
gf	-4.55	kJ/mol	Joback Method
hf	-339.97	kJ/mol	Joback Method
hfus	38.15	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.682		Crippen Method
mcvol	236.330	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1958.00		NIST Webbook
tb	737.23	K	Joback Method
tc	946.74	K	Joback Method
tf	403.06	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.40	J/mol×K	737.23	Joback Method
cpg	677.92	J/mol×K	772.15	Joback Method
cpg	693.36	J/mol×K	807.07	Joback Method
cpg	707.74	J/mol×K	841.99	Joback Method
cpg	721.09	J/mol×K	876.90	Joback Method
cpg	733.44	J/mol×K	911.82	Joback Method
cpg	744.82	J/mol×K	946.74	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=U299846&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