(Phenylthio)acetic acid, 2-ethylcyclohexyl ester

Inchi: InChI=1S/C16H22O2S/c1-2-13-8-6-7-11-15(13)18-16(17)12-19-14-9-4-3-5-10-14/h3-5,9-

InchiKey: ZPOLETLEMOLZDN-UHFFFAOYSA-N

Formula: C16H22O2S

SMILES: CCC1CCCCC1OC(=O)CSc1ccccc1

Mol. weight [g/mol]: 278.41

Physical Properties

Property code	Value	Unit	Source
gf	12.19	kJ/mol	Joback Method
hf	-305.99	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	69.58	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.291		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook
tb	752.11	K	Joback Method
tc	993.31	K	Joback Method
tf	406.20	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.41	J/mol×K	752.11	Joback Method
cpg	677.72	J/mol×K	792.31	Joback Method
cpg	695.38	J/mol×K	832.51	Joback Method
cpg	711.44	J/mol×K	872.71	Joback Method
cpg	725.93	J/mol×K	912.91	Joback Method
cpg	738.88	J/mol×K	953.11	Joback Method
cpg	750.34	J/mol×K	993.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308356&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