(Phenylthio)acetic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C20H26O2S/c21-19(14-23-18-4-2-1-3-5-18)22-7-6-20-11-15-8-16(12-20)10-17

InchiKey: MVJMRHGNZUBBPJ-UHFFFAOYSA-N

Formula: C20H26O2S

SMILES: O=C(CSc1ccccc1)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 330.48

Physical Properties

Property code	Value	Unit	Source
gf	186.08	kJ/mol	Joback Method
hf	-215.39	kJ/mol	Joback Method
hfus	35.59	kJ/mol	Joback Method
hvap	76.81	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.928		Crippen Method
mcvol	260.110	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	2665.00		NIST Webbook
tb	848.81	K	Joback Method
tc	1094.40	K	Joback Method
tf	518.10	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.70	J/mol×K	848.81	Joback Method
cpg	866.74	J/mol×K	889.74	Joback Method
cpg	887.28	J/mol×K	930.67	Joback Method
cpg	907.60	J/mol×K	971.60	Joback Method
cpg	927.98	J/mol×K	1012.53	Joback Method
cpg	948.71	J/mol×K	1053.46	Joback Method
cpg	970.09	J/mol×K	1094.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299958&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