(Phenylthio)acetic acid, cyclobutyl ester

Inchi: InChI=1S/C12H14O2S/c13-12(14-10-5-4-6-10)9-15-11-7-2-1-3-8-11/h1-3,7-8,10H,4-6,9H
InchiKey: LCBNKGBZYHOULH-UHFFFAOYSA-N
Formula: C12H14O2S
SMILES: O=C(CSc1ccccc1)OC1CCC1
Mol. weight [g/mol]: 222.30

Physical Properties

Property code	Value	Unit	Source
gf	10.42	kJ/mol	Joback Method
hf	-190.77	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	60.64	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.874		Crippen Method
mcvol	169.110	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
tb	656.72	K	Joback Method
tc	903.12	K	Joback Method
tf	372.40	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.57	J/mol×K	656.72	Joback Method
cpg	451.82	J/mol×K	697.79	Joback Method
cpg	466.79	J/mol×K	738.85	Joback Method
cpg	480.52	J/mol×K	779.92	Joback Method
cpg	493.09	J/mol×K	820.99	Joback Method
cpg	504.53	J/mol×K	862.06	Joback Method
cpg	514.91	J/mol×K	903.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299955&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