Propanoic acid, 3-phenyl, 2,3-bis-(methylthio), methyl ester

Inchi: InChI=1S/C12H16O2S2/c1-14-12(13)11(16-3)10(15-2)9-7-5-4-6-8-9/h4-8,10-11H,1-3H3
InchiKey: QLUIJBCKOAYTBD-UHFFFAOYSA-N
Formula: C12H16O2S2
SMILES: COC(=O)C(SC)C(SC)c1ccccc1
Mol. weight [g/mol]: 256.38

Physical Properties

Property code	Value	Unit	Source
gf	-9.99	kJ/mol	Joback Method
hf	-226.10	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	66.60	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.995		Crippen Method
mcvol	196.320	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1948.00		NIST Webbook
rinpol	1948.00		NIST Webbook
tb	713.61	K	Joback Method
tc	961.73	K	Joback Method
tf	362.38	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.07	J/mol×K	713.61	Joback Method
cpg	518.12	J/mol×K	754.96	Joback Method
cpg	531.89	J/mol×K	796.32	Joback Method
cpg	544.41	J/mol×K	837.67	Joback Method
cpg	555.68	J/mol×K	879.03	Joback Method
cpg	565.73	J/mol×K	920.38	Joback Method
cpg	574.56	J/mol×K	961.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R121836&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