2-Propenoic acid, 3,3-diphenyl-2-(o-methoxyphenyl)-

Inchi: InChI=1S/C22H18O3/c1-25-19-15-9-8-14-18(19)21(22(23)24)20(16-10-4-2-5-11-16)17-1

InchiKey: RHDBQQXIWBILRU-UHFFFAOYSA-N

Formula: C22H18O3

SMILES: COc1ccccc1C(C(=O)O)=C(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 330.38

CAS: 5129-14-6

Physical Properties

Property code	Value	Unit	Source
gf	154.34	kJ/mol	Joback Method
hf	-98.68	kJ/mol	Joback Method
hfus	38.93	kJ/mol	Joback Method
hvap	98.01	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.739		Crippen Method
mcvol	258.570	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
tb	960.17	K	Joback Method
tc	1206.18	K	Joback Method
tf	529.46	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.13	J/mol×K	960.17	Joback Method
cpg	791.11	J/mol×K	1001.17	Joback Method
cpg	802.11	J/mol×K	1042.17	Joback Method
cpg	812.26	J/mol×K	1083.18	Joback Method
cpg	821.68	J/mol×K	1124.18	Joback Method
cpg	830.50	J/mol×K	1165.18	Joback Method
cpg	838.83	J/mol×K	1206.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129146&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume