Alpha,alpha-diphenyl-beta-propiolactone

Inchi: InChI=1S/C15H12O2/c16-14-15(11-17-14,12-7-3-1-4-8-12)13-9-5-2-6-10-13/h1-10H,11H
InchiKey: KPURDRXLOMYQAS-UHFFFAOYSA-N
Formula: C15H12O2
SMILES: O=C1OCC1(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 224.25
CAS: 16230-71-0

Physical Properties

Property code	Value	Unit	Source
gf	134.69	kJ/mol	Joback Method
hf	-67.69	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	61.23	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.530		Crippen Method
mcvol	171.270	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
tb	701.98	K	Joback Method
tc	982.17	K	Joback Method
tf	444.76	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.28	J/mol×K	701.98	Joback Method
cpg	481.79	J/mol×K	748.68	Joback Method
cpg	498.17	J/mol×K	795.38	Joback Method
cpg	513.70	J/mol×K	842.07	Joback Method
cpg	528.65	J/mol×K	888.77	Joback Method
cpg	543.32	J/mol×K	935.47	Joback Method
cpg	557.98	J/mol×K	982.17	Joback Method

Sources

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=C16230710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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