Ethanone, 2-(2-methylpropoxy)-1,2-diphenyl-

Other names:	Acetophenone, 2-isobutoxy-2-phenyl-
	Benzoin isobutyl ether
	Isobutyl benzoin ether
	Triganol
	Vicure 10
	O-isobutylbenzoin
Inchi:	InChI=1S/C18H20O2/c1-14(2)13-20-18(16-11-7-4-8-12-16)17(19)15-9-5-3-6-10-15/h3-12
InchiKey:	JMVZGKVGQDHWOI-UHFFFAOYSA-N
Formula:	C18H20O2
SMILES:	CC(C)COC(C(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	268.35
CAS:	22499-12-3

Physical Properties

Property code	Value	Unit	Source
gf	86.70	kJ/mol	Joback Method
hf	-197.15	kJ/mol	Joback Method
hfus	26.20	kJ/mol	Joback Method
hvap	68.59	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.283		Crippen Method
mcvol	224.400	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
tb	740.01	K	Joback Method
tc	973.00	K	Joback Method
tf	387.62	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.75	J/mol×K	740.01	Joback Method
cpg	645.05	J/mol×K	778.84	Joback Method
cpg	660.98	J/mol×K	817.67	Joback Method

cpg	675.61	J/mol×K	856.51	Joback Method
cpg	689.01	J/mol×K	895.34	Joback Method
cpg	701.25	J/mol×K	934.17	Joback Method
cpg	712.38	J/mol×K	973.00	Joback Method
dvisc	0.0018115	Pa×s	387.62	Joback Method
dvisc	0.0007711	Pa×s	446.35	Joback Method
dvisc	0.0004004	Pa×s	505.08	Joback Method
dvisc	0.0002383	Pa×s	563.82	Joback Method
dvisc	0.0001564	Pa×s	622.55	Joback Method
dvisc	0.0001104	Pa×s	681.28	Joback Method
dvisc	0.0000823	Pa×s	740.01	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	406.20	K	0.07	NIST Webbook

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=C22499123&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume