

1-Propanone, 1,3,3-triphenyl-

Other names:	Propiophenone, 3,3-diphenyl- 3,3-Diphenylpropiophenone Beta,beta-diphenylpropiophenone
Inchi:	InChI=1S/C21H18O/c22-21(19-14-8-3-9-15-19)16-20(17-10-4-1-5-11-17)18-12-6-2-7-13-
InchiKey:	WYRBITQXPQGTBL-UHFFFAOYSA-N
Formula:	C21H18O
SMILES:	O=C(CC(c1ccccc1)c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	286.37
CAS:	606-86-0

Physical Properties

Property code	Value	Unit	Source
gf	331.81	kJ/mol	Joback Method
hf	114.96	kJ/mol	Joback Method
hfus	30.35	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.091		Crippen Method
mcvol	237.040	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
tb	813.35	K	Joback Method
tc	1073.57	K	Joback Method
tf	440.62	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.79	J/molxK	813.35	Joback Method
cpg	692.31	J/molxK	856.72	Joback Method
cpg	707.29	J/molxK	900.09	Joback Method
cpg	720.87	J/molxK	943.46	Joback Method
cpg	733.20	J/molxK	986.83	Joback Method
cpg	744.43	J/molxK	1030.20	Joback Method

cpg	754.72	J/mol×K	1073.57	Joback Method
dvisc	0.0013118	Paxs	440.62	Joback Method
dvisc	0.0006201	Paxs	502.74	Joback Method
dvisc	0.0003456	Paxs	564.86	Joback Method
dvisc	0.0002163	Paxs	626.98	Joback Method
dvisc	0.0001473	Paxs	689.11	Joback Method
dvisc	0.0001069	Paxs	751.23	Joback Method
dvisc	0.0000815	Paxs	813.35	Joback Method

Sources

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=C606860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/63-472-8/1-Propanone-1-3-3-triphenyl.pdf>

Generated by Cheméo on 2024-04-29 13:11:07.038916027 +0000 UTC m=+16685515.959493338.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.