Beta,beta-diphenylpropiophenone

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

Physical Properties

Property code	Value	Unit	Source
af	0.5754		Cheméo Relay (1.0)
gf	331.81	kJ/mol	Joback Method
hf	130.17	kJ/mol	Cheméo Relay (1.0)
hfus	30.35	kJ/mol	Joback Method
hvap	107.52	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-5.30		Cheméo Relay (1.0)
logp	5.091		Crippen Method
mcvol	237.040	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
tb	646.45	K	Cheméo Relay (1.0)
tc	974.15	K	Cheméo Relay (1.0)
tf	340.69	K	Cheméo Relay (1.0)
vc	0.844	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.79	J/mol×K	813.35	Joback Method
cpg	754.72	J/mol×K	1073.57	Joback Method
cpg	744.43	J/mol×K	1030.20	Joback Method
cpg	733.20	J/mol×K	986.83	Joback Method
cpg	720.87	J/mol×K	943.46	Joback Method

cpg	707.29	J/mol×K	900.09	Joback Method
cpg	692.31	J/mol×K	856.72	Joback Method
dvisc	0.0002163	Pa×s	626.99	Joback Method
dvisc	0.0000815	Pa×s	813.35	Joback Method
dvisc	0.0001069	Pa×s	751.23	Joback Method
dvisc	0.0001473	Pa×s	689.11	Joback Method
dvisc	0.0013118	Pa×s	440.62	Joback Method
dvisc	0.0003456	Pa×s	564.86	Joback Method
dvisc	0.0006201	Pa×s	502.74	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C606860&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
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
ie: Ionization energy
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