4,4'-Diphenoxybenzophenone

Other names: Benzophenone, 4,4'-diphenoxy-
Inchi: InChI=1S/C25H18O3/c26-25(19-11-15-23(16-12-19)27-21-7-3-1-4-8-21)20-13-17-24(18-
InchiKey: BSILAEQTGTZMIW-UHFFFAOYSA-N
Formula: C25H18O3
SMILES: O=C(c1ccc(Oc2ccccc2)cc1)c1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 366.42

Physical Properties

Property code	Value	Unit	Source
af	0.8253		Cheméo Relay (1.0)
gf	251.08	kJ/mol	Joback Method
hf	-22.12	kJ/mol	Cheméo Relay (1.0)
hfus	39.87	kJ/mol	Joback Method
hvap	145.86	kJ/mol	Cheméo Relay (1.0)
ie	7.90	eV	Cheméo Relay (1.0)
log10ws	-7.40		Cheméo Relay (1.0)
logp	6.502		Crippen Method
mcvol	281.380	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
tb	754.11	K	Cheméo Relay (1.0)
tc	1086.25	K	Cheméo Relay (1.0)
tf	403.98	K	Cheméo Relay (1.0)
vc	1.024	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	851.21	J/mol×K	986.79	Joback Method
cpg	863.31	J/mol×K	1031.75	Joback Method
cpg	873.77	J/mol×K	1076.72	Joback Method
cpg	882.72	J/mol×K	1121.68	Joback Method
cpg	890.26	J/mol×K	1166.65	Joback Method
cpg	896.52	J/mol×K	1211.61	Joback Method
cpg	901.62	J/mol×K	1256.58	Joback Method

dvisc	0.0002628	Pa×s	596.62	Joback Method
dvisc	0.0001555	Pa×s	661.65	Joback Method
dvisc	0.0001010	Pa×s	726.68	Joback Method
dvisc	0.0000705	Pa×s	791.71	Joback Method
dvisc	0.0000519	Pa×s	856.73	Joback Method
dvisc	0.0000400	Pa×s	921.76	Joback Method
dvisc	0.0000318	Pa×s	986.79	Joback Method

Sources

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=C14984215&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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