

2,4,5-Triethoxybenzophenone

Other names:	Methanone, phenyl(2,4,5-triethoxyphenyl)-
Inchi:	InChI=1S/C19H22O4/c1-4-21-16-13-18(23-6-3)17(22-5-2)12-15(16)19(20)14-10-8-7-9-11
InchiKey:	ATJSQHQQSASKB-UHFFFAOYSA-N
Formula:	C19H22O4
SMILES:	CCOc1cc(OCC)c(C(=O)c2ccccc2)cc1OCC
Mol. weight [g/mol]:	314.38
CAS:	52199-46-9

Physical Properties

Property code	Value	Unit	Source
gf	-138.89	kJ/mol	Joback Method
hf	-506.08	kJ/mol	Joback Method
hfus	37.04	kJ/mol	Joback Method
hvap	78.40	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.114		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
tb	823.55	K	Joback Method
tc	1043.55	K	Joback Method
tf	510.91	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.74	J/mol×K	823.55	Joback Method
cpg	751.08	J/mol×K	860.22	Joback Method
cpg	765.14	J/mol×K	896.88	Joback Method
cpg	777.93	J/mol×K	933.55	Joback Method
cpg	789.46	J/mol×K	970.21	Joback Method
cpg	799.74	J/mol×K	1006.88	Joback Method
cpg	808.76	J/mol×K	1043.55	Joback Method
dvisc	0.0003600	Pa×s	510.91	Joback Method

dvisc	0.0002237	Pa×s	563.02	Joback Method
dvisc	0.0001507	Pa×s	615.12	Joback Method
dvisc	0.0001080	Pa×s	667.23	Joback Method
dvisc	0.0000812	Pa×s	719.34	Joback Method
dvisc	0.0000635	Pa×s	771.44	Joback Method
dvisc	0.0000512	Pa×s	823.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52199469&Units=SI
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

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

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