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: ATJSQHQJQSASKB-UHFFFAOYSA-N
Formula: C19H22O4
SMILES: CCOc1cc(OCC)c(C(=O)c2ccccc2)cc1OCC
Mol. weight [g/mol]: 314.38

Physical Properties

Property code	Value	Unit	Source
af	0.8462		Cheméo Relay (1.0)
hf	-524.50	kJ/mol	Cheméo Relay (1.0)
hfus	37.04	kJ/mol	Joback Method
hvap	102.34	kJ/mol	Cheméo Relay (1.0)
ie	8.23	eV	Cheméo Relay (1.0)
log10ws	-4.72		Cheméo Relay (1.0)
logp	4.114		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
tb	666.36	K	Cheméo Relay (1.0)
tc	893.78	K	Cheméo Relay (1.0)
tf	342.47	K	Cheméo Relay (1.0)
vc	0.933	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.74	J/mol×K	823.55	Joback Method
cpg	808.76	J/mol×K	1043.55	Joback Method
cpg	799.74	J/mol×K	1006.88	Joback Method
cpg	789.46	J/mol×K	970.21	Joback Method
cpg	777.93	J/mol×K	933.55	Joback Method
cpg	765.14	J/mol×K	896.88	Joback Method
cpg	751.08	J/mol×K	860.22	Joback Method
dvisc	0.0001080	Pa×s	667.23	Joback Method

dvisc	0.0000512	Pa×s	823.55	Joback Method
dvisc	0.0000635	Pa×s	771.44	Joback Method
dvisc	0.0000812	Pa×s	719.34	Joback Method
dvisc	0.0003600	Pa×s	510.91	Joback Method
dvisc	0.0001507	Pa×s	615.12	Joback Method
dvisc	0.0002237	Pa×s	563.02	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=C52199469&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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