DESOXYANISOIN

Other names:	Deoxy-4-anisoin
	Ethanone, 1,2-bis(4-methoxyphenyl)-
	Acetophenone, 4'-methoxy-2-(p-methoxyphenyl)-
	Deoxy-p-anisoin
	Deoxyanisoin
	4-Methoxybenzyl 4-methoxyphenyl ketone
	4,4'-Dimethoxydeoxybenzoin
	1,2-Bis(4-methoxyphenyl)ethanone
	1,2-Bis(p-methoxyphenyl)ethanone
	1,2-Di-p-anisylethanone
	4'-Methoxy-2-(p-methoxyphenyl)acetophenone
	4-Methoxybenzyl 4'-methoxyphenyl ketone
	p-Methoxybenzyl p-methoxyphenyl ketone
Inchi:	InChI=1S/C16H16O3/c1-18-14-7-3-12(4-8-14)11-16(17)13-5-9-15(19-2)10-6-13/h3-10H,1
InchiKey:	SICBLYCPRWNHHP-UHFFFAOYSA-N
Formula:	C16H16O3
SMILES:	COc1ccc(CC(=O)c2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	256.30

Physical Properties

Property code	Value	Unit	Source
hf	-274.07	kJ/mol	Cheméo Relay (1.0)
hfus	28.48	kJ/mol	Joback Method
hvap	98.11	kJ/mol	Cheméo Relay (1.0)
ie	7.83	eV	Cheméo Relay (1.0)
log10ws	-4.18		Cheméo Relay (1.0)
logp	3.129		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
tb	648.22	K	Cheméo Relay (1.0)
tf	371.30	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	543.43	J/mol×K	727.51	Joback Method
cpg	558.78	J/mol×K	766.07	Joback Method
cpg	572.96	J/mol×K	804.63	Joback Method
cpg	586.00	J/mol×K	843.18	Joback Method
cpg	597.92	J/mol×K	881.74	Joback Method
cpg	608.73	J/mol×K	920.30	Joback Method
cpg	618.46	J/mol×K	958.86	Joback Method
dvisc	0.0007122	Pa×s	442.35	Joback Method
dvisc	0.0004327	Pa×s	489.88	Joback Method
dvisc	0.0002872	Pa×s	537.40	Joback Method
dvisc	0.0002037	Pa×s	584.93	Joback Method
dvisc	0.0001521	Pa×s	632.46	Joback Method
dvisc	0.0001184	Pa×s	679.98	Joback Method
dvisc	0.0000951	Pa×s	727.51	Joback Method

Sources

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=C120445&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point