

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

CAS:

120-44-5

Physical Properties

Property code	Value	Unit	Source
gf	-49.52	kJ/mol	Joback Method
hf	-300.47	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.129		Crippen Method
mcvol	202.090	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
tb	727.51	K	Joback Method
tc	958.86	K	Joback Method
tf	442.35	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.43	J/molxK	727.51	Joback Method
cpg	558.78	J/molxK	766.07	Joback Method
cpg	572.96	J/molxK	804.63	Joback Method
cpg	586.00	J/molxK	843.18	Joback Method
cpg	597.92	J/molxK	881.74	Joback Method
cpg	608.73	J/molxK	920.30	Joback Method
cpg	618.46	J/molxK	958.86	Joback Method
dvisc	0.0007122	Paxs	442.35	Joback Method
dvisc	0.0004327	Paxs	489.88	Joback Method
dvisc	0.0002872	Paxs	537.40	Joback Method
dvisc	0.0002037	Paxs	584.93	Joback Method
dvisc	0.0001521	Paxs	632.46	Joback Method
dvisc	0.0001184	Paxs	679.98	Joback Method
dvisc	0.0000951	Paxs	727.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120445&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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