4-Benzyloxy-3-methoxyacetophenone

Other names: 4'-Benzyloxy-3'-methoxyacetophenone
Acetophenone, 4'-(benzyloxy)-3'-methoxy-
Ethanone, 1-(3-methoxy-4-(phenylmethoxy)phenyl)-
Inchi: InChI=1S/C16H16O3/c1-12(17)14-8-9-15(16(10-14)18-2)19-11-13-6-4-3-5-7-13/h3-10H,1
InchiKey: HRUAWSQBQLYDKH-UHFFFAOYSA-N
Formula: C16H16O3
SMILES: COc1cc(C(C)=O)ccc1OCc1ccccc1
Mol. weight [g/mol]: 256.30
CAS: 1835-11-6

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	-4.48		Crippen Method
logp	3.477		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	m3/kmol	Joback Method

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

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1835116&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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