2-Propen-1-one, 3-(4-methoxyphenyl)-1-phenyl-

Other names: Chalcone, 4-methoxy-
Phenyl p-methoxystyryl ketone
3-(4-Methoxyphenyl)-1-phenyl-2-propen-1-one
4-Methoxychalcone
4'-Methoxybenzylideneacetophenone
(4-Methoxybenzylidene)acetophenone
p-Methoxystyryl phenyl ketone
4-Methoxystyryl phenyl ketone
(p-Methoxybenzylidene)acetophenone
1-Phenyl-3-(4-methoxyphenyl)-2-propen-1-one
NSC 11866

Inchi: InChI=1S/C16H14O2/c1-18-15-10-7-13(8-11-15)9-12-16(17)14-5-3-2-4-6-14/h2-12H,1H3

InchiKey: XUFXKBJMCRJATM-FMIVXFBMSA-N

Formula: C16H14O2

SMILES: COc1ccc(C=CC(=O)c2ccccc2)cc1

Mol. weight [g/mol]: 238.28

CAS: 959-33-1

Physical Properties

Property code	Value	Unit	Source
chs	-8138.70	kJ/mol	NIST Webbook
gf	145.33	kJ/mol	Joback Method
hf	-39.56	kJ/mol	Joback Method
hfs	-195.00	kJ/mol	NIST Webbook
hfus	27.88	kJ/mol	Joback Method
hvap	65.54	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.591		Crippen Method
mcvol	191.920	ml/mol	McGowan Method
pc	2477.65	kPa	Joback Method
tb	704.27	K	Joback Method
tc	947.48	K	Joback Method
tf	402.52	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.64	J/mol×K	704.27	Joback Method
cpg	510.01	J/mol×K	744.80	Joback Method
cpg	524.16	J/mol×K	785.34	Joback Method
cpg	537.15	J/mol×K	825.87	Joback Method
cpg	549.06	J/mol×K	866.41	Joback Method
cpg	559.97	J/mol×K	906.94	Joback Method
cpg	569.95	J/mol×K	947.48	Joback Method
dvisc	0.0010692	Pa×s	402.52	Joback Method
dvisc	0.0005864	Pa×s	452.81	Joback Method
dvisc	0.0003626	Pa×s	503.10	Joback Method
dvisc	0.0002447	Pa×s	553.39	Joback Method
dvisc	0.0001763	Pa×s	603.69	Joback Method
dvisc	0.0001336	Pa×s	653.98	Joback Method
dvisc	0.0001053	Pa×s	704.27	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C959331&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase 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