

Acetophenone, 4',4'''-ethylenedi-

Other names:	4,4'-Diacetyldiphenylethane Ethanone, 1,1'-(1,2-ethanediyl-di-4,1-phenylene)bis-
Inchi:	InChI=1S/C18H18O2/c1-13(19)17-9-5-15(6-10-17)3-4-16-7-11-18(12-8-16)14(2)20/h5-12
InchiKey:	ZSLCVLSXAOHWBQ-UHFFFAOYSA-N
Formula:	C18H18O2
SMILES:	CC(=O)c1ccc(CCC2ccc(C(C)=O)cc2)cc1
Mol. weight [g/mol]:	266.33
CAS:	793-06-6

Physical Properties

Property code	Value	Unit	Source
gf	48.40	kJ/mol	Joback Method
hf	-189.89	kJ/mol	Joback Method
hfus	32.88	kJ/mol	Joback Method
hvap	75.03	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	3.877		Crippen Method
mcvol	220.100	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
tb	782.30	K	Joback Method
tc	1016.75	K	Joback Method
tf	470.36	K	Joback Method
vc	0.840	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.58	J/mol×K	782.30	Joback Method
cpg	628.55	J/mol×K	821.37	Joback Method
cpg	642.32	J/mol×K	860.45	Joback Method
cpg	654.98	J/mol×K	899.52	Joback Method
cpg	666.59	J/mol×K	938.60	Joback Method
cpg	677.22	J/mol×K	977.67	Joback Method
cpg	686.93	J/mol×K	1016.75	Joback Method

dvisc	0.0010211	Pa×s	470.36	Joback Method
dvisc	0.0006065	Pa×s	522.35	Joback Method
dvisc	0.0003958	Pa×s	574.34	Joback Method
dvisc	0.0002773	Pa×s	626.33	Joback Method
dvisc	0.0002052	Pa×s	678.32	Joback Method
dvisc	0.0001585	Pa×s	730.31	Joback Method
dvisc	0.0001267	Pa×s	782.30	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=C793066&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

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