

Ethanone, 1-(4-ethoxyphenyl)-

Other names:	4'-Ethoxyacetophenone p-Ethoxyacetophenone 4-Ethoxyacetophenone 4-Ethoxyphenylethanone Acetophenone, p-ethoxy- Acetophenone, 4'-ethoxy- 1-(4-Ethoxyphenyl)ethanone 1-(4-ethoxyphenyl)ethan-1-one
Inchi:	InChI=1S/C10H12O2/c1-3-12-10-6-4-9(5-7-10)8(2)11/h4-7H,3H2,1-2H3
InchiKey:	YJFNFQHMJQJCPRG-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCOc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	164.20
CAS:	1676-63-7

Physical Properties

Property code	Value	Unit	Source
gf	-97.82	kJ/mol	Joback Method
hf	-269.47	kJ/mol	Joback Method
hfus	18.10	kJ/mol	Joback Method
hvap	49.95	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.288		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
tb	536.15	K	Joback Method
tc	749.95	K	Joback Method
tf	313.56	K	Joback Method
vc	0.511	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.27	J/mol×K	536.15	Joback Method

cpg	313.54	J/molxK	571.78	Joback Method
cpg	326.10	J/molxK	607.42	Joback Method
cpg	337.97	J/molxK	643.05	Joback Method
cpg	349.15	J/molxK	678.68	Joback Method
cpg	359.66	J/molxK	714.31	Joback Method
cpg	369.52	J/molxK	749.95	Joback Method
dvisc	0.0017515	Paxs	313.56	Joback Method
dvisc	0.0010200	Paxs	350.66	Joback Method
dvisc	0.0006587	Paxs	387.76	Joback Method
dvisc	0.0004592	Paxs	424.86	Joback Method
dvisc	0.0003392	Paxs	461.95	Joback Method
dvisc	0.0002621	Paxs	499.05	Joback Method
dvisc	0.0002099	Paxs	536.15	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	541.70	K	101.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1676637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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