Ethanone, 1-(4-ethylphenyl)-

Other names:	Acetophenone, 4'-ethyl-
	p-Acetylethylbenzene
	p-Ethylacetophenone
	p-Ethylphenyl methyl ketone
	4'-Ethylacetophenone
	4-Ethylacetophenone
	1-(4-Ethylphenyl)ethanone
Inchi:	InChI=1S/C10H12O/c1-3-9-4-6-10(7-5-9)8(2)11/h4-7H,3H2,1-2H3
InchiKey:	NODGRWCMFMEGJH-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CCc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	148.20
CAS:	937-30-4

Physical Properties

Property code	Value	Unit	Source
gf	7.18	kJ/mol	Joback Method
hf	-137.25	kJ/mol	Joback Method
hfus	16.91	kJ/mol	Joback Method
hvap	47.54	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.452		Crippen Method
mcvol	129.570	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
rinpol	1281.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1273.80		NIST Webbook
rinpol	1281.00		NIST Webbook

ripol	1867.00		NIST Webbook
ripol	1867.00		NIST Webbook
tb	512.00 ± 2.00	K	NIST Webbook
tc	729.82	K	Joback Method
tf	248.90 ± 0.25	K	NIST Webbook
tf	252.60 ± 2.00	K	NIST Webbook
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.66	J/mol×K	513.73	Joback Method
cpg	290.22	J/mol×K	549.75	Joback Method
cpg	303.00	J/mol×K	585.76	Joback Method
cpg	315.02	J/mol×K	621.78	Joback Method
cpg	326.32	J/mol×K	657.79	Joback Method
cpg	336.91	J/mol×K	693.81	Joback Method
cpg	346.84	J/mol×K	729.82	Joback Method
dvisc	0.0012729	Pa×s	328.40	Joback Method
dvisc	0.0022588	Pa×s	291.33	Joback Method
dvisc	0.0008058	Pa×s	365.46	Joback Method
dvisc	0.0005549	Pa×s	402.53	Joback Method
dvisc	0.0004070	Pa×s	439.60	Joback Method
dvisc	0.0003132	Pa×s	476.66	Joback Method
dvisc	0.0002503	Pa×s	513.73	Joback Method
hvapt	42.20	kJ/mol	331.00	NIST Webbook
hvapt	39.80	kJ/mol	358.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.20	K	2.70	NIST Webbook

Sources

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=C937304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume