Ethanone, 1-[4-(1-methylethyl)phenyl]-

Other names:	Acetophenone, 4'-isopropyl-
	p-Isopropylacetophenone
	Cuminone
	4-Isopropylacetophenone
	4'-Isopropylacetophenone
	(4-Isopropylphenyl)ethanone
	1-[4-(1-methylethyl)phenyl]ethan-1-one
Inchi:	InChI=1S/C11H14O/c1-8(2)10-4-6-11(7-5-10)9(3)12/h4-8H,1-3H3
InchiKey:	PDLCCNYKIIUWHA-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CC(=O)c1ccc(C(C)C)cc1
Mol. weight [g/mol]:	162.23
CAS:	645-13-6

Physical Properties

Property code	Value	Unit	Source
gf	13.16	kJ/mol	Joback Method
hf	-163.17	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	49.38	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.013		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2808.38	kPa	Joback Method
rinpol	1585.00		NIST Webbook
tb	527.20	K	NIST Webbook
tc	753.50	K	Joback Method
tf	287.60	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.92	J/mol×K	536.17	Joback Method

cpg	336.78	J/mol×K	572.39	Joback Method
cpg	350.78	J/mol×K	608.61	Joback Method
cpg	363.93	J/mol×K	644.84	Joback Method
cpg	376.27	J/mol×K	681.06	Joback Method
cpg	387.82	J/mol×K	717.28	Joback Method
cpg	398.64	J/mol×K	753.50	Joback Method
dvisc	0.0029954	Pa×s	287.60	Joback Method
dvisc	0.0014787	Pa×s	329.03	Joback Method
dvisc	0.0008548	Pa×s	370.46	Joback Method
dvisc	0.0005518	Pa×s	411.89	Joback Method
dvisc	0.0003858	Pa×s	453.31	Joback Method
dvisc	0.0002864	Pa×s	494.74	Joback Method
dvisc	0.0002227	Pa×s	536.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C645136&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume