

2'-Ethylacetophenone

Inchi:	InChI=1S/C10H12O/c1-3-9-6-4-5-7-10(9)8(2)11/h4-7H,3H2,1-2H3
InchiKey:	VLILFBZIVHDKIJ-UHFFFAOYSA-N
Formula:	C10H12O
SMILES:	CCc1ccccc1C(C)=O
Mol. weight [g/mol]:	148.20

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	1210.00		NIST Webbook
tb	513.73	K	Joback Method
tc	729.82	K	Joback Method
tf	291.33	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.66	J/molxK	513.73	Joback Method
cpg	290.22	J/molxK	549.75	Joback Method
cpg	303.00	J/molxK	585.76	Joback Method
cpg	315.02	J/molxK	621.78	Joback Method
cpg	326.32	J/molxK	657.79	Joback Method
cpg	336.91	J/molxK	693.81	Joback Method
cpg	346.84	J/molxK	729.82	Joback Method
dvisc	0.0022588	Paxs	291.33	Joback Method
dvisc	0.0012729	Paxs	328.40	Joback Method

dvisc	0.0008058	Paxs	365.46	Joback Method
dvisc	0.0005549	Paxs	402.53	Joback Method
dvisc	0.0004070	Paxs	439.60	Joback Method
dvisc	0.0003132	Paxs	476.66	Joback Method
dvisc	0.0002503	Paxs	513.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R553476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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