2-ethylacetophenone

Other names: 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
CAS: 2142-64-5

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
tb	513.73	K	Joback Method
tc	729.82	K	Joback Method
tf	254.20 ± 1.00	K	NIST Webbook
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.84	J/mol×K	729.82	Joback Method
cpg	336.91	J/mol×K	693.81	Joback Method
cpg	326.32	J/mol×K	657.79	Joback Method
cpg	315.02	J/mol×K	621.78	Joback Method
cpg	303.00	J/mol×K	585.76	Joback Method
cpg	290.22	J/mol×K	549.75	Joback Method
cpg	276.66	J/mol×K	513.73	Joback Method
dvisc	0.0022588	Pa×s	291.33	Joback Method

dvisc	0.0002503	Pa×s	513.73	Joback Method
dvisc	0.0003132	Pa×s	476.66	Joback Method
dvisc	0.0004070	Pa×s	439.60	Joback Method
dvisc	0.0005549	Pa×s	402.53	Joback Method
dvisc	0.0008058	Pa×s	365.46	Joback Method
dvisc	0.0012729	Pa×s	328.40	Joback Method
hvapt	52.80	kJ/mol	380.00	NIST Webbook

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=C2142645&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume