3-Ethylbenzophenone

Inchi: InChI=1S/C15H14O/c1-2-12-7-6-10-14(11-12)15(16)13-8-4-3-5-9-13/h3-11H,2H2,1H3
InchiKey: FVSYHKJWZIKKDM-UHFFFAOYSA-N
Formula: C15H14O
SMILES: CCc1cccc(C(=O)c2ccccc2)c1
Mol. weight [g/mol]: 210.27
CAS: 66067-43-4

Physical Properties

Property code	Value	Unit	Source
gf	161.69	kJ/mol	Joback Method
hf	-3.92	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	60.94	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.480		Crippen Method
mcvol	176.260	ml/mol	McGowan Method
pc	2635.25	kPa	Joback Method
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
tb	654.81	K	Joback Method
tc	897.12	K	Joback Method
tf	374.10	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.18	J/mol×K	654.81	Joback Method
cpg	456.23	J/mol×K	695.20	Joback Method
cpg	471.04	J/mol×K	735.58	Joback Method
cpg	484.66	J/mol×K	775.97	Joback Method
cpg	497.18	J/mol×K	816.35	Joback Method
cpg	508.66	J/mol×K	856.74	Joback Method
cpg	519.18	J/mol×K	897.12	Joback Method

dvisc	0.0016640	Pa×s	374.10	Joback Method
dvisc	0.0009227	Pa×s	420.88	Joback Method
dvisc	0.0005757	Pa×s	467.67	Joback Method
dvisc	0.0003914	Pa×s	514.45	Joback Method
dvisc	0.0002837	Pa×s	561.24	Joback Method
dvisc	0.0002161	Pa×s	608.02	Joback Method
dvisc	0.0001712	Pa×s	654.81	Joback Method

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=C66067434&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
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