Isocaprophenone

Inchi: InChI=1S/C12H16O/c1-10(2)8-9-12(13)11-6-4-3-5-7-11/h3-7,10H,8-9H2,1-2H3
InchiKey: WRJZDDJYWWJLIS-UHFFFAOYSA-N
Formula: C12H16O
SMILES: CC(C)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 176.25

Physical Properties

Property code	Value	Unit	Source
gf	31.21	kJ/mol	Joback Method
hf	-172.34	kJ/mol	Joback Method
hfus	18.95	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.305		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1396.00		NIST Webbook
tb	554.07	K	Joback Method
tc	766.69	K	Joback Method
tf	286.35	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.74	J/mol×K	554.07	Joback Method
cpg	384.70	J/mol×K	589.51	Joback Method
cpg	399.69	J/mol×K	624.94	Joback Method
cpg	413.76	J/mol×K	660.38	Joback Method
cpg	426.95	J/mol×K	695.82	Joback Method
cpg	439.29	J/mol×K	731.25	Joback Method
cpg	450.82	J/mol×K	766.69	Joback Method
dvisc	0.0041343	Pa×s	286.35	Joback Method
dvisc	0.0018071	Pa×s	330.97	Joback Method

dvisc	0.0009615	Pa×s	375.59	Joback Method
dvisc	0.0005850	Pa×s	420.21	Joback Method
dvisc	0.0003915	Pa×s	464.83	Joback Method
dvisc	0.0002811	Pa×s	509.45	Joback Method
dvisc	0.0002129	Pa×s	554.07	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323196&Units=SI

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