Acetyl cymene

Other names: Acetophenone, 2'-methyl-5'-isopropyl
Inchi: InChI=1S/C12H16O/c1-8(2)11-6-5-9(3)12(7-11)10(4)13/h5-8H,1-4H3
InchiKey: LVNVQCXLRILPCM-UHFFFAOYSA-N
Formula: C12H16O
SMILES: CC(=O)c1cc(C(C)C)ccc1C
Mol. weight [g/mol]: 176.25

Physical Properties

Property code	Value	Unit	Source
gf	11.95	kJ/mol	Joback Method
hf	-195.28	kJ/mol	Joback Method
hfus	18.18	kJ/mol	Joback Method
hvap	52.26	kJ/mol	Joback Method
log10ws	-3.79		Crippen Method
logp	3.321		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1381.00		NIST Webbook
rinpol	1358.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1928.00		NIST Webbook
tb	564.03	K	Joback Method
tc	778.76	K	Joback Method
tf	311.39	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.54	J/mol×K	564.03	Joback Method
cpg	383.90	J/mol×K	599.82	Joback Method
cpg	398.39	J/mol×K	635.61	Joback Method
cpg	412.05	J/mol×K	671.39	Joback Method

cpg	424.91	J/mol×K	707.18	Joback Method
cpg	436.99	J/mol×K	742.97	Joback Method
cpg	448.33	J/mol×K	778.76	Joback Method
dvisc	0.0021912	Pa×s	311.39	Joback Method
dvisc	0.0011633	Pa×s	353.50	Joback Method
dvisc	0.0007067	Pa×s	395.60	Joback Method
dvisc	0.0004725	Pa×s	437.71	Joback Method
dvisc	0.0003391	Pa×s	479.82	Joback Method
dvisc	0.0002567	Pa×s	521.92	Joback Method
dvisc	0.0002026	Pa×s	564.03	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R409364&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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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