2,3,5,6-Tetramethylacetophenone

Other names:	2',3',5',6'-Tetramethylacetophenone
	Acetophenone, 2',3',5',6'-tetramethyl-
	Ethanone, 1-(2,3,5,6-tetramethylphenyl)-
	Methyl duryl ketone
	1,2,4,5-Tetramethyl-3-acetylbenzene
Inchi:	InChI=1S/C12H16O/c1-7-6-8(2)10(4)12(9(7)3)11(5)13/h6H,1-5H3
InchiKey:	JCNRSGPJXDRATR-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	CC(=O)c1c(C)c(C)cc(C)c1C
Mol. weight [g/mol]:	176.25
CAS:	2142-79-2

Physical Properties

Property code	Value	Unit	Source
gf	-4.87	kJ/mol	Joback Method
hf	-212.94	kJ/mol	Joback Method
hfus	20.92	kJ/mol	Joback Method
hvap	53.98	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.123		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	574.43	K	Joback Method
tc	786.68	K	Joback Method
tf	351.43	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	367.59	J/mol×K	574.43	Joback Method
cpg	432.74	J/mol×K	751.31	Joback Method
cpg	421.08	J/mol×K	715.93	Joback Method
cpg	408.75	J/mol×K	680.56	Joback Method

cpg	395.74	J/mol×K	645.18	Joback Method
cpg	382.02	J/mol×K	609.81	Joback Method
cpg	443.73	J/mol×K	786.68	Joback Method
dvisc	0.0002076	Pa×s	574.43	Joback Method
dvisc	0.0002492	Pa×s	537.26	Joback Method
dvisc	0.0003073	Pa×s	500.10	Joback Method
dvisc	0.0003919	Pa×s	462.93	Joback Method
dvisc	0.0005215	Pa×s	425.76	Joback Method
dvisc	0.0007328	Pa×s	388.60	Joback Method
dvisc	0.0011068	Pa×s	351.43	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=C2142792&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume