2,4,6-Tri-isopropylacetophenone

Other names:	2',4',6'-Triisopropylacetophenone
	Ethanone, 1-[2,4,6-tris(1-methylethyl)phenyl]-
	Acetophenone, 2',4',6'-triisopropyl-
	Acetophenone: 2',4',6'-triisopropyl
	1-[2,4,6-tris(1-methylethyl)phenyl]ethan-1-one
Inchi:	InChI=1S/C17H26O/c1-10(2)14-8-15(11(3)4)17(13(7)18)16(9-14)12(5)6/h8-12H,1-7H3
InchiKey:	SGRDDUKVLKWIBZ-UHFFFAOYSA-N
Formula:	C17H26O
SMILES:	CC(=O)c1c(C(C)C)cc(C(C)C)cc1C(C)C
Mol. weight [g/mol]:	246.39
CAS:	2234-14-2

Physical Properties

Property code	Value	Unit	Source
gf	39.54	kJ/mol	Joback Method
hf	-320.51	kJ/mol	Joback Method
hfus	23.69	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-5.69		Crippen Method
logp	5.259		Crippen Method
mcvol	228.200	ml/mol	McGowan Method
pc	1629.85	kPa	Joback Method
tb	682.53	K	Joback Method
tc	889.78	K	Joback Method
tf	350.26	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.44	J/mol×K	682.53	Joback Method
cpg	708.46	J/mol×K	855.24	Joback Method

cpg	694.03	J/mol×K	820.70	Joback Method
cpg	678.64	J/mol×K	786.16	Joback Method
cpg	662.26	J/mol×K	751.61	Joback Method
cpg	644.87	J/mol×K	717.07	Joback Method
cpg	721.98	J/mol×K	889.78	Joback Method
dvisc	0.0001092	Pa×s	682.53	Joback Method
dvisc	0.0001442	Pa×s	627.15	Joback Method
dvisc	0.0002010	Pa×s	571.77	Joback Method
dvisc	0.0003009	Pa×s	516.39	Joback Method
dvisc	0.0004962	Pa×s	461.02	Joback Method
dvisc	0.0009381	Pa×s	405.64	Joback Method
dvisc	0.0021690	Pa×s	350.26	Joback Method

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=C2234142&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
ie:	Ionization energy
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