

METHANONE, PHENYL(2,4,6-TRIMETHYLPHENYL)-

Other names:	2,4,6-Trimethylbenzophenone
	2,4,6-Trimetilbenzofenon
	Ketone, mesityl phenyl
	Mesityl phenyl ketone
	Mesitylene, 2-benzoyl-
	Methanone, phenyl(2,4,6-trimethylphenyl)-
Inchi:	InChI=1S/C16H16O/c1-11-9-12(2)15(13(3)10-11)16(17)14-7-5-4-6-8-14/h4-10H,1-3H3
InchiKey:	HPAFOABSQZMTHE-UHFFFAOYSA-N
Formula:	C16H16O
SMILES:	Cc1cc(C)c(C(=O)c2ccccc2)c(C)c1
Mol. weight [g/mol]:	224.30

Physical Properties

Property code	Value	Unit	Source
af	0.5869		Cheméo Relay (1.0)
gf	150.85	kJ/mol	Joback Method
hf	-34.18	kJ/mol	Cheméo Relay (1.0)
hfus	25.71	kJ/mol	Joback Method
hvap	87.16	kJ/mol	Cheméo Relay (1.0)
ie	8.00	eV	NIST Webbook
ie	8.32	eV	NIST Webbook
log10ws	-4.76		Cheméo Relay (1.0)
logp	3.843		Crippen Method
mcvol	190.350	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	605.44	K	Cheméo Relay (1.0)
tc	861.82	K	Cheméo Relay (1.0)
tf	329.41	K	Cheméo Relay (1.0)
vc	0.694	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.90	J/mol×K	687.65	Joback Method

cpg	506.00	J/mol×K	727.48	Joback Method
cpg	520.93	J/mol×K	767.30	Joback Method
cpg	534.74	J/mol×K	807.13	Joback Method
cpg	547.50	J/mol×K	846.96	Joback Method
cpg	559.24	J/mol×K	886.78	Joback Method
cpg	570.04	J/mol×K	926.61	Joback Method
dvisc	0.0010758	Pa×s	410.41	Joback Method
dvisc	0.0006609	Pa×s	456.62	Joback Method
dvisc	0.0004440	Pa×s	502.82	Joback Method
dvisc	0.0003190	Pa×s	549.03	Joback Method
dvisc	0.0002412	Pa×s	595.24	Joback Method
dvisc	0.0001899	Pa×s	641.44	Joback Method
dvisc	0.0001544	Pa×s	687.65	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C954165&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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

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