2,2,2-Triphenylacetophenone

Other names:	2,2,2-Triphenylacetophenone
	Benzopinacolone
	«beta»-Benzopinacolone
	Ethanone, tetraphenyl-
	1,2,2,2-Tetraphenyl-1-ethanone
	«omega»,«omega»,«omega»-Triphenylacetophenone
	Phenyl trityl ketone
	Tetraphenylethanone
	1,2,2,2-Tetraphenylethanone
Inchi:	InChI=1S/C26H20O/c27-25(21-13-5-1-6-14-21)26(22-15-7-2-8-16-22,23-17-9-3-10-18-23
InchiKey:	CFBBKHROQRFCNZ-UHFFFAOYSA-N
Formula:	C26H20O
SMILES:	O=C(c1ccccc1)C(c1ccccc1)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	348.44

Physical Properties

Property code	Value	Unit	Source
af	0.6034		Cheméo Relay (1.0)
chs	-13310.00	kJ/mol	NIST Webbook
gf	491.60	kJ/mol	Joback Method
hf	281.91	kJ/mol	Cheméo Relay (1.0)
hfus	33.45	kJ/mol	Joback Method
hvap	100.47	kJ/mol	Cheméo Relay (1.0)
ie	8.16	eV	Cheméo Relay (1.0)
log10ws	-7.19		Cheméo Relay (1.0)
logp	5.904		Crippen Method
mcvol	283.730	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
tb	703.19	K	Cheméo Relay (1.0)
tc	1061.78	K	Cheméo Relay (1.0)
tf	508.02	K	Cheméo Relay (1.0)
vc	0.990	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.47	J/mol×K	951.64	Joback Method
cpg	940.36	J/mol×K	1236.07	Joback Method
cpg	928.39	J/mol×K	1188.67	Joback Method
cpg	916.35	J/mol×K	1141.26	Joback Method
cpg	903.93	J/mol×K	1093.86	Joback Method
cpg	890.84	J/mol×K	1046.45	Joback Method
cpg	876.79	J/mol×K	999.05	Joback Method
dvisc	0.0000956	Pa×s	746.23	Joback Method
dvisc	0.0000360	Pa×s	951.64	Joback Method
dvisc	0.0000474	Pa×s	883.17	Joback Method
dvisc	0.0000653	Pa×s	814.70	Joback Method
dvisc	0.0005338	Pa×s	540.81	Joback Method
dvisc	0.0001510	Pa×s	677.75	Joback Method
dvisc	0.0002645	Pa×s	609.28	Joback Method

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C466375&Units=SI

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

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

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