Pindone

Other names:	1,3-Indandione, 2-pivaloyl-
	1H-Indene-1,3(2H)-dione, 2-(2,2-dimethyl-1-oxopropyl)-
	2-(2,2-Dimethyl-1-oxopropyl)-1H-indene-1,3-(2H)-dione
	2-(Trimethylacetyl)-1,3-indandione
	2-(Trimetil-acetil)-indan-1,3-dione
	2-Pivaloyl-1,3-indandione
	2-Pivaloyl-indaan-1,3-dion
	2-Pivaloyl-indan-1,3-dion
	2-Pivaloylindan-1,3-dione
	2-Pivaloylindane-1,3-dione
	2-Pivalyl-1,3-indandione
	Chemrat
	Latka 333
	NSC 31211
	Pindon
	Pivacin
	Pival
	Pivaldion
	Pivaldione
	Pivalyl
	Pivalyl Valone
	Pivalyl indan-1,3-dione
	Pivalyn
	Tri-ban
	UN 2472
Inchi:	InChI=1S/C14H14O3/c1-14(2,3)13(17)10-11(15)8-6-4-5-7-9(8)12(10)16/h4-7,10H,1-3H3
InchiKey:	RZKYEQDPDZUERB-UHFFFAOYSA-N
Formula:	C14H14O3
SMILES:	CC(C)(C)C(=O)C1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	230.26
CAS:	83-26-1

Physical Properties

Property code	Value	Unit	Source
gf	-140.73	kJ/mol	Joback Method
hf	-431.16	kJ/mol	Joback Method

hfus	17.01	kJ/mol	Joback Method
hvap	63.55	kJ/mol	Joback Method
log10ws	-4.11		Aqueous Solubility Prediction Method
logp	2.297		Crippen Method
mcvol	178.210	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1783.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
rinpol	1783.00		NIST Webbook
tb	744.40	K	Joback Method
tc	997.15	K	Joback Method
tf	383.00 ± 0.20	K	NIST Webbook
tf	382.70 ± 0.20	K	NIST Webbook
tf	382.88 ± 0.20	K	NIST Webbook
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.12	J/mol×K	744.40	Joback Method
cpg	528.73	J/mol×K	786.52	Joback Method
cpg	543.03	J/mol×K	828.65	Joback Method
cpg	556.06	J/mol×K	870.77	Joback Method
cpg	567.85	J/mol×K	912.90	Joback Method
cpg	578.46	J/mol×K	955.02	Joback Method
cpg	587.92	J/mol×K	997.15	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C83261&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume