2-Benzoyl-1,3-indanedione

Other names:	1,3-Indandione, 2-benzoyl-
	Benzoylindandione
	2-Benzoyl-1,3-indandione
	1H-Indene-1,3(2H)-dione, 2-benzoyl-
Inchi:	InChI=1S/C16H10O3/c17-14(10-6-2-1-3-7-10)13-15(18)11-8-4-5-9-12(11)16(13)19/h1-9,
InchiKey:	UURMMRCWXJLUKF-UHFFFAOYSA-N
Formula:	C16H10O3
SMILES:	O=C(c1ccccc1)C1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]:	250.25
CAS:	1785-95-1

Physical Properties

Property code	Value	Unit	Source
gf	-14.32	kJ/mol	Joback Method
hf	-227.16	kJ/mol	Joback Method
hfus	23.64	kJ/mol	Joback Method
hvap	71.58	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.565		Crippen Method
mcvol	182.630	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	820.07	K	Joback Method
tc	1093.68	K	Joback Method
tf	539.75	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	525.79	J/mol×K	820.07	Joback Method
cpg	539.69	J/mol×K	865.67	Joback Method
cpg	552.02	J/mol×K	911.27	Joback Method
cpg	562.84	J/mol×K	956.87	Joback Method
cpg	572.18	J/mol×K	1002.47	Joback Method

cpg	580.08	J/mol×K	1048.08	Joback Method
cpg	586.58	J/mol×K	1093.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1785951&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume