2(2-Acetyl-1-phenylethyl) 1,3-indandione

Inchi: InChI=1S/C19H16O3/c1-12(20)11-16(13-7-3-2-4-8-13)17-18(21)14-9-5-6-10-15(14)19(17
InchiKey: KJULKZCUOFDKHU-UHFFFAOYSA-N
Formula: C19H16O3
SMILES: CC(=O)CC(c1ccccc1)C1C(=O)c2ccccc2C1=O
Mol. weight [g/mol]: 292.33
CAS: 1785-98-4

Physical Properties

Property code	Value	Unit	Source
gf	8.50	kJ/mol	Joback Method
hf	-294.36	kJ/mol	Joback Method
hfus	27.89	kJ/mol	Joback Method
hvap	77.87	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.445		Crippen Method
mcvol	224.900	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
tb	888.27	K	Joback Method
tc	1149.18	K	Joback Method
tf	558.56	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.38	J/mol×K	888.27	Joback Method
cpg	707.74	J/mol×K	931.76	Joback Method
cpg	720.47	J/mol×K	975.24	Joback Method
cpg	731.64	J/mol×K	1018.73	Joback Method
cpg	741.29	J/mol×K	1062.21	Joback Method
cpg	749.47	J/mol×K	1105.70	Joback Method
cpg	756.23	J/mol×K	1149.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1785984&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