1,2-Indandione, 3,3-dimethyl-

Other names: 1H-Indene-1,2(3H)-dione, 3,3-dimethyl-
3,3-Dimethyl-1,2-indanedione
Inchi: InChI=1S/C11H10O2/c1-11(2)8-6-4-3-5-7(8)9(12)10(11)13/h3-6H,1-2H3
InchiKey: XEBYAZZOVDAJAQ-UHFFFAOYSA-N
Formula: C11H10O2
SMILES: CC1(C)C(=O)C(=O)c2ccccc21
Mol. weight [g/mol]: 174.20
CAS: 20651-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-45.40	kJ/mol	Joback Method
hf	-232.67	kJ/mol	Joback Method
hfus	8.75	kJ/mol	Joback Method
hvap	50.27	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
log10ws	-2.20		Crippen Method
logp	1.730		Crippen Method
mcvol	134.370	ml/mol	McGowan Method
pc	3407.89	kPa	Joback Method
tb	625.36	K	Joback Method
tc	884.97	K	Joback Method
tf	430.95	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.74	J/mol×K	625.36	Joback Method
cpg	353.59	J/mol×K	668.63	Joback Method
cpg	367.62	J/mol×K	711.90	Joback Method
cpg	380.97	J/mol×K	755.16	Joback Method
cpg	393.79	J/mol×K	798.43	Joback Method

cpg	406.21	J/mol×K	841.70	Joback Method
cpg	418.38	J/mol×K	884.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20651881&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
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