2-Phenylindane-1,3-dione

Other names:

1H-Indene-1,3(2H)-dione, 2-phenyl-
Athrombon
Bindan
Danedion
Danilon
Danilone
Diadilan
Dindevan
Dineval
Diophindane
Emandion
Emandione
Fenhydren
Fenilin
Fenindion
Hedulin
1,3-Indandione, 2-phenyl-
Indema
Indion
Indon
Phenhydren
Phenillin
2-Phenyl-1,3-diketohydrindene
Phenylen
Phenylin
2-Phenylindandione
2-Phenyl-1,3-indandione
Phenylindanedione
2-Phenyl-1,3-indanedione
Phenylindione
PID
Pindione
Rectadione
Theradione
Tromazal
Trombol
Eridione
Phenyline
Phenyllin
2-Phenylindan-1,3-dione

	2-Phenyl-1H-indene-1,3(2H)-dione
	Cronodione
	Hemolidione
	Thrombasal
	1,3(2H)-Indenedione, 2-phenyl-
Inchi:	InChI=1S/C15H10O2/c16-14-11-8-4-5-9-12(11)15(17)13(14)10-6-2-1-3-7-10/h1-9,13H
InchiKey:	NFBAXHOPROOJAW-UHFFFAOYSA-N
Formula:	C15H10O2
SMILES:	O=C1c2ccccc2C(=O)C1c1ccccc1
Mol. weight [g/mol]:	222.24

Physical Properties

Property code	Value	Unit	Source
hf	-68.67	kJ/mol	Cheméo Relay (1.0)
hfus	19.45	kJ/mol	Joback Method
hvap	78.12	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-3.99		Cheméo Relay (1.0)
logp	2.849		Crippen Method
mcvol	166.970	ml/mol	McGowan Method
rinpol	2055.00		NIST Webbook
rinpol	346.66		NIST Webbook
rinpol	347.47		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	2055.00		NIST Webbook
tb	627.33	K	Cheméo Relay (1.0)
tf	446.48	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.07	J/mol×K	743.32	Joback Method
cpg	477.06	J/mol×K	789.44	Joback Method
cpg	491.51	J/mol×K	835.56	Joback Method
cpg	504.46	J/mol×K	881.68	Joback Method
cpg	515.95	J/mol×K	927.80	Joback Method
cpg	526.02	J/mol×K	973.92	Joback Method

cpg	534.71	J/mol×K	1020.04	Joback Method

Sources

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=C83125&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point