1H-Indene-1,3(2H)-dione, 2-(diphenylacetyl)-

Other names:	1H-Indene-1,3(2H)-dione, 2-(diphenylacetyl)-
	1,3-Indandione, 2-(diphenylacetyl)-
	Didandin
	Didion
	Dipaxin
	Diphacin
	Diphacinone
	Diphenacin
	Diphenadion
	Diphenandione
	Oragulant
	Ratindan
	Ratindan 1
	Solvan
	U 1363
	2-(Diphenylacetyl)-1,3-diketohydrindene
	2-(Diphenylacetyl)-1,3-indandione
	Diphac
	Promar
	PID
	Ramik
	URI 788
	2-(Diphenylacetyl)-1H-indene-1,3-(2H)-dione
	2-(Diphenylacetyl)indan-1,3-dione
	2-Diphenyl-acetyl-indan-1,3-dion
	Kill-ko rat killer
	NSC 9138
Inchi:	InChI=1S/C23H16O3/c24-21-17-13-7-8-14-18(17)22(25)20(21)23(26)19(15-9-3-1-4-10-1
InchiKey:	JYGLAHSAISAEAL-UHFFFAOYSA-N
Formula:	C23H16O3
SMILES:	O=C1c2ccccc2C(=O)C1C(=O)C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	340.38

Physical Properties

Property code	Value	Unit	Source
hfus	32.29	kJ/mol	Joback Method

hvap	110.10	kJ/mol	Cheméo Relay (1.0)
log10ws	-5.04		Cheméo Relay (1.0)
logp	4.083		Crippen Method
mcvol	257.500	ml/mol	McGowan Method
rinpol	2934.00		NIST Webbook
rinpol	2934.00		NIST Webbook
tf	432.56	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.63	J/mol×K	1006.47	Joback Method
cpg	828.41	J/mol×K	1053.29	Joback Method
cpg	838.39	J/mol×K	1100.11	Joback Method
cpg	846.70	J/mol×K	1146.92	Joback Method
cpg	853.43	J/mol×K	1193.74	Joback Method
cpg	858.69	J/mol×K	1240.56	Joback Method
cpg	862.61	J/mol×K	1287.38	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C82666&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point