Diphenadione

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]:	340.37
CAS:	82-66-6

Physical Properties

Property code	Value	Unit	Source

gf	154.59	kJ/mol	Joback Method
hf	-140.39	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.083		Crippen Method
mcvol	257.500	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	2934.00		NIST Webbook
rinpol	2934.00		NIST Webbook
tb	1006.47	K	Joback Method
tc	1287.38	K	Joback Method
tf	630.06	K	Joback Method
vc	0.971	m3/kmol	Joback Method

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

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume