Chlorophacinone

Other names:

1H-Indene-1,3(2H)-dione, 2-[(4-chlorophenyl)phenylacetyl]-
1,3-Indandione, 2-[(p-chlorophenyl)phenylacetyl]-
Chlorodiphacinone
Chlorophenacone
Chlorphacinone
Chlorphenacone
Drat
LM 91
Raticide-Caid
2-[(p-Chlorophenyl)phenylacetyl]-1,3-indandione
Actosin C
Afnor
Caid
Chloorfacinon
2(2-(4-Chloor-fenyl-2-fenyl)-acetyl)-indaan-1,3-dion
Chlorfacinon
2(2-(4-Chlorophenyl)-2-phenylacetyl)indan-1,3-dione
2-((4-Chlorophenyl)phenylacetyl)-1H-indene-1,3(2H)-dione
Chlorphacinon
2(2-(4-Chlor-phenyl-2-phenyl)acetyl)indan-1,3-dione
((4-Chlorphenyl)-1-phenyl)-acetyl-1,3-indandion
1-(4-Chlorphenyl)-1-phenyl-acetyl-indan-1,3-dion
2(2-(4-Cloro-fenil-2fenil)-acetil)indan-1,3-dione
Lepit
Liphadione
Microzul
Muriol
2-(2-Phenyl-2-(4-chlorophenyl)acetyl)-1,3-indandione
Ramucide
Ranac
Ratomet
Rozol
Saviac
Topitox
Indandione, 2-((p-chlorophenyl)phenylacetyl)-
Indene-1,3(2H)-dione, 2-((4-chlorophenyl)phenylacetyl)-
Partox
Sakarat special
Skaterpax
Ratindan 3

	Redentin
	Raviac
	Chlorophacinon
Inchi:	InChI=1S/C23H15ClO3/c24-16-12-10-15(11-13-16)19(14-6-2-1-3-7-14)23(27)20-21(25)1
InchiKey:	UDHXJZHVNHGCEC-UHFFFAOYSA-N
Formula:	C23H15ClO3
SMILES:	O=C1c2ccccc2C(=O)C1C(=O)C(c1ccccc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	374.82
CAS:	3691-35-8

Physical Properties

Property code	Value	Unit	Source
gf	133.03	kJ/mol	Joback Method
hf	-167.60	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	94.09	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	4.736		Crippen Method
mcvol	269.740	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
tb	1048.88	K	Joback Method
tc	1331.51	K	Joback Method
tf	418.14 ± 0.20	K	NIST Webbook
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.26	J/mol×K	1048.88	Joback Method
cpg	842.11	J/mol×K	1095.99	Joback Method
cpg	850.22	J/mol×K	1143.09	Joback Method
cpg	856.70	J/mol×K	1190.20	Joback Method
cpg	861.64	J/mol×K	1237.30	Joback Method
cpg	865.15	J/mol×K	1284.41	Joback Method
cpg	867.33	J/mol×K	1331.51	Joback Method
hfust	34.54	kJ/mol	416.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3691358&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
hfust:	Enthalpy of fusion at a given temperature
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