

Anisindione

Other names:	1H-Indene-1,3(2H)-dione, 2-(4-methoxyphenyl)- 1,3-Indandione, 2-(p-methoxyphenyl)- Anisin indandione 2-p-Anisyl-1,3-indandione 2-(p-Methoxyphenyl)-1,3-indandione 2-(4-Methoxyphenyl)-1H-indene-1,3(2H)-dione 2-(p-Methoxyphenyl)indane-1,3-dione Miradon SPE 2792 Unidone Andion
Inchi:	InChI=1S/C16H12O3/c1-19-11-8-6-10(7-9-11)14-15(17)12-4-2-3-5-13(12)16(14)18/h2-9,
InchiKey:	XRCFXMGQEVUZFC-UHFFFAOYSA-N
Formula:	C16H12O3
SMILES:	<chem>COc1ccc(C2C(=O)c3ccccc3C2=O)cc1</chem>
Mol. weight [g/mol]:	252.26
CAS:	117-37-3

Physical Properties

Property code	Value	Unit	Source
gf	-0.03	kJ/mol	Joback Method
hf	-258.27	kJ/mol	Joback Method
hfus	22.84	kJ/mol	Joback Method
hvap	67.90	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.858		Crippen Method
mvol	186.930	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	2273.00		NIST Webbook
tb	793.60	K	Joback Method
tc	1059.11	K	Joback Method
tf	524.57	K	Joback Method
vc	0.705	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.33	J/mol×K	793.60	Joback Method
cpg	554.80	J/mol×K	837.85	Joback Method
cpg	568.72	J/mol×K	882.10	Joback Method
cpg	581.06	J/mol×K	926.35	Joback Method
cpg	591.85	J/mol×K	970.60	Joback Method
cpg	601.07	J/mol×K	1014.86	Joback Method
cpg	608.73	J/mol×K	1059.11	Joback Method

Sources

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=C117373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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