2-(3,4-DIMETHOXYBENZYLIDENE)-1,3-INDANDIO

Other names: 2-(3,4-Dimethoxybenzylidene)-1,3-indandione
Inchi: InChI=1S/C18H14O4/c1-21-15-8-7-11(10-16(15)22-2)9-14-17(19)12-5-3-4-6-13(12)18(14
InchiKey: OVHSLRSKIAKFOH-UHFFFAOYSA-N
Formula: C18H14O4
SMILES: COc1ccc(C=C2C(=O)c3ccccc3C2=O)cc1OC
Mol. weight [g/mol]: 294.31

Physical Properties

Property code	Value	Unit	Source
hfus	28.07	kJ/mol	Joback Method
log10ws	-4.47		Cheméo Relay (1.0)
logp	3.166		Crippen Method
mcvol	216.680	ml/mol	McGowan Method
rinpol	2525.00		NIST Webbook
tb	687.78	K	Cheméo Relay (1.0)
tf	444.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.80	J/mol×K	878.07	Joback Method
cpg	655.32	J/mol×K	920.89	Joback Method
cpg	667.26	J/mol×K	963.72	Joback Method
cpg	677.63	J/mol×K	1006.54	Joback Method
cpg	686.40	J/mol×K	1049.36	Joback Method
cpg	693.56	J/mol×K	1092.18	Joback Method
cpg	699.10	J/mol×K	1135.01	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58161743&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
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