Flavone

Other names:	2-Phenyl-4-chromone
	2-Phenyl-4H-1-benzopyran-4-one
	2-Phenyl-4H-1-benzopyran-4-one (flavone)
	2-Phenyl-4H-benzopyran-4-one
	2-Phenyl-«gamma»-benzopyrone
	2-Phenyl-Â«gammaÂ»-benzopyrone
	2-Phenylbenzopyran-4-one
	2-Phenylchromone
	4H-1-Benzopyran-4-one, 2-phenyl-
	Asmacoril
	Chromocor
	Cromaril
	NSC 19028
	Phenylchromone
Inchi:	InChI=1S/C15H10O2/c16-13-10-15(11-6-2-1-3-7-11)17-14-9-5-4-8-12(13)14/h1-10H
InchiKey:	VHBFFQKBGNRLFZ-UHFFFAOYSA-N
Formula:	C15H10O2
SMILES:	O=c1cc(-c2ccccc2)oc2ccccc12
Mol. weight [g/mol]:	222.24
CAS:	525-82-6

Physical Properties

Property code	Value	Unit	Source
hfus	20.32	kJ/mol	Energetics of flavone and flavanone
hsub	108.20 ± 1.70	kJ/mol	NIST Webbook
log10ws	-9.04		Crippen Method
logp	3.460		Crippen Method
mcvol	166.970	ml/mol	McGowan Method
rinpol	2148.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2150.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.32	kJ/mol	369.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C525826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of flavone, 6-methoxyflavone and anthracene in supercritical CO2 with/without a co-solvent of ethanol correlated by using a newly proposed entropy-based solubility parameter:	https://www.doi.org/10.1016/j.fluid.2016.05.009
Measurement and correlation of vapor-liquid distribution coefficients of [illegible] dioxide - ethanol - water systems:	https://www.doi.org/10.1016/j.fluid.2019.02.015
Energetics of flavone and flavanone:	https://www.doi.org/10.1016/j.jct.2009.06.022

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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