Flavanone

Other names:	2,3-Dihydro-2-phenyl-4H-1-benzopyran-4-one
	2,3-Dihydro-2-phenyl-4H-1-benzopyran-4-one (flavanone)
	2,3-dihydroflavone
	2-Phenyl-4-chromanone
	4-Flavanone
	4H-1-Benzopyran-4-one, 2,3-dihydro-2-phenyl-
Inchi:	InChI=1S/C15H12O2/c16-13-10-15(11-6-2-1-3-7-11)17-14-9-5-4-8-12(13)14/h1-9,15H,10
InchiKey:	ZONYXWQDUYMKFB-UHFFFAOYSA-N
Formula:	C15H12O2
SMILES:	O=C1CC(c2ccccc2)Oc2ccccc21
Mol. weight [g/mol]:	224.25
CAS:	487-26-3

Physical Properties

Property code	Value	Unit	Source
gf	130.55	kJ/mol	Joback Method
hf	-94.40	kJ/mol	Joback Method
hfus	21.04	kJ/mol	Energetics of flavone and flavanone
hvap	63.04	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.393		Crippen Method
mcvol	171.270	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
tb	706.72	K	Joback Method
tc	976.76	K	Joback Method
tf	433.38	K	Joback Method
vc	0.636	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	467.58	J/mol×K	706.72	Joback Method
cpg	484.71	J/mol×K	751.73	Joback Method

cpg	500.29	J/mol×K	796.73	Joback Method
cpg	514.38	J/mol×K	841.74	Joback Method
cpg	527.06	J/mol×K	886.74	Joback Method
cpg	538.42	J/mol×K	931.75	Joback Method
cpg	548.52	J/mol×K	976.76	Joback Method

Sources

Energetics of flavone and flavanone:	https://www.doi.org/10.1016/j.jct.2009.06.022
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=C487263&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume