

2H-1-Benzopyran, 3,4-dihydro-2-phenyl-

Other names:	Flavan 2-Phenylchroman 3,4-Dihydro-2-phenyl-2H-1-benzopyran
Inchi:	InChI=1S/C15H14O/c1-2-6-12(7-3-1)15-11-10-13-8-4-5-9-14(13)16-15/h1-9,15H,10-11H
InchiKey:	QOLIPNRNLBQTAU-UHFFFAOYSA-N
Formula:	C15H14O
SMILES:	<chem>c1ccc(C2CCc3ccccc3O2)cc1</chem>
Mol. weight [g/mol]:	210.27
CAS:	494-12-2

Physical Properties

Property code	Value	Unit	Source
gf	253.14	kJ/mol	Joback Method
hf	43.30	kJ/mol	Joback Method
hfus	26.31	kJ/mol	Joback Method
hvap	58.79	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.753		Crippen Method
mcvol	169.700	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	638.90	K	Joback Method
tc	897.38	K	Joback Method
tf	365.16	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.61	J/molxK	638.90	Joback Method
cpg	517.78	J/molxK	854.30	Joback Method
cpg	504.83	J/molxK	811.22	Joback Method
cpg	490.66	J/molxK	768.14	Joback Method
cpg	475.15	J/molxK	725.06	Joback Method
cpg	458.17	J/molxK	681.98	Joback Method

cpg	529.63	J/mol×K	897.38	Joback Method
dvisc	0.0002943	Paxs	638.90	Joback Method
dvisc	0.0003595	Paxs	593.28	Joback Method
dvisc	0.0004540	Paxs	547.65	Joback Method
dvisc	0.0005983	Paxs	502.03	Joback Method
dvisc	0.0008332	Paxs	456.41	Joback Method
dvisc	0.0012487	Paxs	410.78	Joback Method
dvisc	0.0020706	Paxs	365.16	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C494122&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

Latest version available from:

<https://www.chemeo.com/cid/75-192-6/2H-1-Benzopyran-3-4-dihydro-2-phenyl.pdf>

Generated by Cheméo on 2024-05-01 14:28:28.447417143 +0000 UTC m=+16862957.367994459.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.