2H-1-Benzopyran, 6,7-dimethoxy-2,2-dimethyl-

Other names:	Ageratochromene
	Precocene 2
	Precocene II
	PRICOCENE II
	6,7-Dimethoxy-2,2-dimethyl-2H-benzo(b)pyran
	6,7-dimethoxy-2,2-dimethyl-(2H)-benzopyran (Precocene II)
	6,7-dimethoxy-2,2-dimethyl2H-1-benzopyran
Inchi:	InChI=1S/C13H16O3/c1-13(2)6-5-9-7-11(14-3)12(15-4)8-10(9)16-13/h5-8H,1-4H3
InchiKey:	PTIDGSWTMLSGAH-UHFFFAOYSA-N
Formula:	C13H16O3
SMILES:	COc1cc2c(cc1OC)OC(C)(C)C=C2
Mol. weight [g/mol]:	220.26
CAS:	644-06-4

Physical Properties

Property code	Value	Unit	Source
gf	-80.90	kJ/mol	Joback Method
hf	-366.31	kJ/mol	Joback Method
hfus	23.61	kJ/mol	Joback Method
hvap	57.35	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	2.888		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1683.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1659.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1634.00		NIST Webbook
rinpol	1656.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2373.00		NIST Webbook
ripol	2396.00		NIST Webbook
ripol	2412.00		NIST Webbook
tb	620.66	K	Joback Method
tc	846.08	K	Joback Method

tf	410.36	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.73	J/mol×K	620.66	Joback Method
cpg	458.28	J/mol×K	658.23	Joback Method
cpg	473.01	J/mol×K	695.80	Joback Method
cpg	487.06	J/mol×K	733.37	Joback Method
cpg	500.52	J/mol×K	770.94	Joback Method
cpg	513.50	J/mol×K	808.51	Joback Method
cpg	526.13	J/mol×K	846.08	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C644064&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ripol: Polar retention indices

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