2H-1-Benzopyran, 7-methoxy-2,2-dimethyl-

Other names:	2H-1-Benzopyran, 7-methoxy-2,2-dimethyl-
	Demethoxyageratochromene
	6-Demethoxyageratochromene
	7-Methoxy-2,2-dimethylchromene
	Precocene 1
	Pricocene I
	2H-1-Benzopyran, 2,2-dimethyl-7-methoxy-
	2,2-Dimethyl-7-methoxy-2H-1-benzopyran
	NSC 318791
Inchi:	InChI=1S/C12H14O2/c1-12(2)7-6-9-4-5-10(13-3)8-11(9)14-12/h4-8H,1-3H3
InchiKey:	CPTJXGLQLVPIGP-UHFFFAOYSA-N
Formula:	C12H14O2
SMILES:	COc1ccc2c(c1)OC(C)(C)C=C2
Mol. weight [g/mol]:	190.24

Physical Properties

Property code	Value	Unit	Source
hfus	20.22	kJ/mol	Joback Method
ie	7.56	eV	Cheméo Relay (1.0)
logp	2.879		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
rinpol	1428.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1471.60		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1471.60		NIST Webbook
rinpol	1478.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2075.00		NIST Webbook
ripol	2068.00		NIST Webbook
ripol	2046.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.74	J/mol×K	570.38	Joback Method
cpg	385.17	J/mol×K	609.05	Joback Method
cpg	399.60	J/mol×K	647.71	Joback Method
cpg	413.17	J/mol×K	686.38	Joback Method
cpg	426.03	J/mol×K	725.05	Joback Method
cpg	438.31	J/mol×K	763.72	Joback Method
cpg	450.16	J/mol×K	802.38	Joback Method

Sources

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):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17598026&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

hfus: Enthalpy of fusion at standard conditions

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices