Precocene I

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
CAS:	17598-02-6

Physical Properties

Property code	Value	Unit	Source
gf	25.31	kJ/mol	Joback Method
hf	-201.98	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	52.05	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	2.879		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1471.60		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1467.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1471.60		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1478.00		NIST Webbook
ripol	2046.00		NIST Webbook
ripol	2068.00		NIST Webbook

ripol	2075.00		NIST Webbook
tb	570.38	K	Joback Method
tc	802.38	K	Joback Method
tf	364.34	K	Joback Method
vc	0.572	m3/kmol	Joback Method

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

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

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