6-vinyl-7-methoxy-2,2-dimethyl-chromene

Inchi: InChI=1S/C14H16O2/c1-5-10-8-11-6-7-14(2,3)16-13(11)9-12(10)15-4/h5-9H,1H2,2-4H3
InchiKey: RRUFTPKJXNXMAE-UHFFFAOYSA-N
Formula: C14H16O2
SMILES: C=Cc1cc2c(cc1OC)OC(C)(C)C=C2
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
gf	120.36	kJ/mol	Joback Method
hf	-129.30	kJ/mol	Joback Method
hfus	23.74	kJ/mol	Joback Method
hvap	56.50	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.522		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
pc	2441.06	kPa	Joback Method
ripol	2354.00		NIST Webbook
ripol	2354.00		NIST Webbook
tb	617.80	K	Joback Method
tc	846.69	K	Joback Method
tf	397.64	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.44	J/mol×K	617.80	Joback Method
cpg	461.31	J/mol×K	655.95	Joback Method
cpg	476.28	J/mol×K	694.10	Joback Method
cpg	490.48	J/mol×K	732.25	Joback Method
cpg	504.07	J/mol×K	770.39	Joback Method
cpg	517.19	J/mol×K	808.54	Joback Method
cpg	529.99	J/mol×K	846.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R239531&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume