2,2-dimethyl-6-vinylchroman-4-one

Inchi: InChI=1S/C13H14O2/c1-4-9-5-6-12-10(7-9)11(14)8-13(2,3)15-12/h4-7H,1,8H2,2-3H3
InchiKey: OKOIYQKVDCIBFR-UHFFFAOYSA-N
Formula: C13H14O2
SMILES: C=Cc1ccc2c(c1)C(=O)CC(C)(C)O2
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
gf	74.02	kJ/mol	Joback Method
hf	-160.45	kJ/mol	Joback Method
hfus	18.64	kJ/mol	Joback Method
hvap	55.15	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.073		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
pc	2778.85	kPa	Joback Method
rinpol	1582.00		NIST Webbook
rinpol	1582.00		NIST Webbook
tb	636.18	K	Joback Method
tc	882.87	K	Joback Method
tf	419.08	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.98	J/mol×K	636.18	Joback Method
cpg	436.26	J/mol×K	677.29	Joback Method
cpg	451.61	J/mol×K	718.41	Joback Method
cpg	466.20	J/mol×K	759.52	Joback Method
cpg	480.16	J/mol×K	800.64	Joback Method
cpg	493.68	J/mol×K	841.75	Joback Method
cpg	506.91	J/mol×K	882.87	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=R405124&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume