6-(1'-Hydroxyethyl)-2,2-dimethylchromene

Inchi: InChI=1S/C13H16O2/c1-9(14)10-4-5-12-11(8-10)6-7-13(2,3)15-12/h4-9,14H,1-3H3
InchiKey: ICIIMFRGWJJFIH-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: CC(O)c1ccc2c(c1)C=CC(C)(C)O2
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	-0.53	kJ/mol	Joback Method
hf	-247.91	kJ/mol	Joback Method
hfus	22.19	kJ/mol	Joback Method
hvap	68.16	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	2.924		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
ripol	2383.00		NIST Webbook
ripol	2383.00		NIST Webbook
tb	662.58	K	Joback Method
tc	879.45	K	Joback Method
tf	399.20	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.11	J/mol×K	662.58	Joback Method
cpg	461.73	J/mol×K	698.72	Joback Method
cpg	474.66	J/mol×K	734.87	Joback Method
cpg	487.04	J/mol×K	771.01	Joback Method
cpg	499.01	J/mol×K	807.16	Joback Method
cpg	510.71	J/mol×K	843.30	Joback Method
cpg	522.28	J/mol×K	879.45	Joback Method

Sources

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=U360290&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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