

7-Hydroxy-2,2-dimethylchromene

Inchi:	InChI=1S/C11H12O2/c1-11(2)6-5-8-3-4-9(12)7-10(8)13-11/h3-7,12H,1-2H3
InchiKey:	GFXPDSJDSLEZTB-UHFFFAOYSA-N
Formula:	C11H12O2
SMILES:	CC1(C)C=Cc2ccc(O)cc2O1
Mol. weight [g/mol]:	176.21

Physical Properties

Property code	Value	Unit	Source
gf	-23.10	kJ/mol	Joback Method
hf	-214.96	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	59.77	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.576		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
ripol	2266.00		NIST Webbook
ripol	2266.00		NIST Webbook
tb	600.72	K	Joback Method
tc	850.50	K	Joback Method
tf	430.04	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.05	J/mol×K	600.72	Joback Method
cpg	363.39	J/mol×K	642.35	Joback Method
cpg	375.73	J/mol×K	683.98	Joback Method
cpg	387.34	J/mol×K	725.61	Joback Method
cpg	398.49	J/mol×K	767.24	Joback Method
cpg	409.44	J/mol×K	808.87	Joback Method
cpg	420.47	J/mol×K	850.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R239546&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

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

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