3,4-Dihydrocoumarin, 4,4-dimethyl-6-hydroxy-

Other names:	Coumarin-6-ol, 3,4-dihydro-4,4-dimethyl- 6-Hydroxy-4,4-dimethyl-3H-cromen-2-one
Inchi:	InChI=1S/C11H12O3/c1-11(2)6-10(13)14-9-4-3-7(12)5-8(9)11/h3-5,12H,6H2,1-2H3
InchiKey:	UKYURFSTLUGMPH-UHFFFAOYSA-N
Formula:	C11H12O3
SMILES:	CC1(C)CC(=O)Oc2ccc(O)cc21
Mol. weight [g/mol]:	192.21
CAS:	29423-72-1

Physical Properties

Property code	Value	Unit	Source
gf	-175.65	kJ/mol	Joback Method
hf	-410.44	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.979		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1336.00		NIST Webbook
tb	669.38	K	Joback Method
tc	929.10	K	Joback Method
tf	497.50	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.45	J/mol×K	669.38	Joback Method
cpg	407.45	J/mol×K	712.67	Joback Method
cpg	420.79	J/mol×K	755.95	Joback Method
cpg	433.71	J/mol×K	799.24	Joback Method
cpg	446.45	J/mol×K	842.53	Joback Method
cpg	459.26	J/mol×K	885.82	Joback Method

cpg	472.39	J/mol×K	929.10	Joback Method

Sources

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=C29423721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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