2H-1-Benzopyran-2-one, 3,4-dihydro-6-methyl-

Other names:	Hydrocoumarin, 6-methyl-
	3,4-Dihydro-6-methylcoumarin
	6-Methyl-3,4-dihydrocoumarin
	6-Methylhydrocoumarin
	3,4-dihydro-6-methyl-2H-1-benzopyran-2-one
Inchi:	InChI=1S/C10H10O2/c1-7-2-4-9-8(6-7)3-5-10(11)12-9/h2,4,6H,3,5H2,1H3
InchiKey:	TWAXWQHDMDUHDN-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	Cc1ccc2c(c1)CCC(=O)O2
Mol. weight [g/mol]:	162.19
CAS:	92-47-7

Physical Properties

Property code	Value	Unit	Source
gf	-25.88	kJ/mol	Joback Method
hf	-218.86	kJ/mol	Joback Method
hfus	17.37	kJ/mol	Joback Method
hvap	50.61	kJ/mol	Joback Method
log10ws	-2.54		Crippen Method
logp	1.847		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook
tb	575.29	K	Joback Method
tc	822.59	K	Joback Method
tf	367.37	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.49	J/mol×K	575.29	Joback Method
cpg	311.02	J/mol×K	616.51	Joback Method

cpg	324.61	J/mol×K	657.72	Joback Method
cpg	337.27	J/mol×K	698.94	Joback Method
cpg	349.04	J/mol×K	740.16	Joback Method
cpg	359.93	J/mol×K	781.37	Joback Method
cpg	369.97	J/mol×K	822.59	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=C92477&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