1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-, (R)-

Other names: Isocoumarin, 3,4-dihydro-8-hydroxy-6-methoxy-3-methyl-, (R)-(-)-
(-)-6-Methoxymellein
6-Methoxymellein

Inchi: InChI=1S/C11H12O4/c1-6-3-7-4-8(14-2)5-9(12)10(7)11(13)15-6/h4-6,12H,3H2,1-2H3/t6-

InchiKey: AIFNAMVERSBWPS-LURJTMIESA-N

Formula: C11H12O4

SMILES: COc1cc(O)c2c(c1)CC(C)OC2=O

Mol. weight [g/mol]: 208.21

CAS: 13410-15-6

Physical Properties

Property code	Value	Unit	Source
gf	-284.79	kJ/mol	Joback Method
hf	-569.37	kJ/mol	Joback Method
hfus	28.00	kJ/mol	Joback Method
hvap	67.95	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.502		Crippen Method
mcvol	150.410	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
rinpol	1848.40		NIST Webbook
tb	696.54	K	Joback Method
tc	942.94	K	Joback Method
tf	508.35	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.47	J/mol×K	696.54	Joback Method
cpg	434.24	J/mol×K	737.61	Joback Method
cpg	447.12	J/mol×K	778.67	Joback Method
cpg	459.16	J/mol×K	819.74	Joback Method
cpg	470.40	J/mol×K	860.81	Joback Method

cpg	480.91	J/mol×K	901.88	Joback Method
cpg	490.72	J/mol×K	942.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13410156&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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