1H-2-Benzopyran-1-one, 3,4-dihydro-8-hydroxy-3-methyl-

Other names: Isocoumarin, 3,4-dihydro-8-hydroxy-3-methyl-
3,4-Dihydro-8-hydroxy-3-methylisocoumarin
Mellein
(.+/-.)-Mellein
8-Hydroxy-3-methyl-3,4-dihydro-1H-isochromen-1-one
3,4-Dihydro-8-hydroxy-3-methyl-1H-2-benzopyran-1-one, (.+/-.)-
3,4-Dihydro-8-hydroxy-3-methyl-(1H)-2-benzopyran-1-one
Isocoumarin, 3,4-dihydro-8-hydroxy-3-methyl, (.+/-.)-
3-Methyl-8-hydroxy-3,4-dihydro-1H-2-benzopyran-1-one

Inchi: InChI=1S/C10H10O3/c1-6-5-7-3-2-4-8(11)9(7)10(12)13-6/h2-4,6,11H,5H2,1H3

InchiKey: KWILGNNWGSNMPA-UHFFFAOYSA-N

Formula: C10H10O3

SMILES: CC1Cc2cccc(O)c2C(=O)O1

Mol. weight [g/mol]: 178.18

CAS: 1200-93-7

Physical Properties

Property code	Value	Unit	Source
gf	-178.58	kJ/mol	Joback Method
hf	-405.04	kJ/mol	Joback Method
hfus	24.61	kJ/mol	Joback Method
hvap	62.65	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.494		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
ripol	2432.00		NIST Webbook
ripol	2432.00		NIST Webbook
tb	646.26	K	Joback Method
tc	901.80	K	Joback Method
tf	462.33	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.99	J/mol×K	646.26	Joback Method
cpg	361.46	J/mol×K	688.85	Joback Method
cpg	373.97	J/mol×K	731.44	Joback Method
cpg	385.61	J/mol×K	774.03	Joback Method
cpg	396.45	J/mol×K	816.62	Joback Method
cpg	406.60	J/mol×K	859.21	Joback Method
cpg	416.13	J/mol×K	901.80	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1200937&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume