Hydrocoumarin

Other names:	1,2-Benzodihydropyrone 1,2-benzodihydropyrone (dihydrocoumarin) 2-Chromanone 2H-1-Benzopyran-2-one, 3,4-dihydro- 3,4-Dihydro-2H-1-benzopyran-2-one 3,4-Dihydrocoumarin Benzodihydropyrone Benzopyranone, dihydro- Chroman, 2-oxo- Coumarin, 3,4-dihydro- Dihydrobenzopyrone Hydrocinnamic acid, o-hydroxy-, «delta»-lactone Melilotin Melilotine Melilotol NCI-C55890 USAF DO-12 dihydrocoumarin
Inchi:	InChI=1S/C9H8O2/c10-9-6-5-7-3-1-2-4-8(7)11-9/h1-4H,5-6H2
InchiKey:	VMUXSMXIQBNMGZ-UHFFFAOYSA-N
Formula:	C9H8O2
SMILES:	O=C1CCc2ccccc2O1
Mol. weight [g/mol]:	148.16
CAS:	119-84-6

Physical Properties

Property code	Value	Unit	Source
gf	-24.67	kJ/mol	Joback Method
hf	-186.75	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	69.90 ± 0.50	kJ/mol	NIST Webbook
log10ws	-2.06		Crippen Method
logp	1.538		Crippen Method
mcvol	110.490	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	1350.00		NIST Webbook
rinpol	1392.00		NIST Webbook

rinpol	1359.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1350.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2290.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2286.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2314.00		NIST Webbook
tb	545.20	K	NIST Webbook
tc	799.04	K	Joback Method
tf	343.58	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.63	J/mol×K	547.43	Joback Method
cpg	265.51	J/mol×K	589.36	Joback Method
cpg	278.43	J/mol×K	631.30	Joback Method
cpg	290.42	J/mol×K	673.23	Joback Method
cpg	301.51	J/mol×K	715.17	Joback Method
cpg	311.73	J/mol×K	757.10	Joback Method
cpg	321.13	J/mol×K	799.04	Joback Method
hvapt	69.90	kJ/mol	298.15	Experimental and computational thermochemistry of the isomers: Chromanone, 3-isochromanone, and dihydrocoumarin

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental and computational thermochemistry of the isomers: chromanone, 3-isochromanone, and dihydrocoumarin:	https://www.doi.org/10.1016/j.jct.2008.08.012
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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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