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

Other names: 1,2-Benzodihydropyrone
1,2-benzodihydropyrone (dihydrocoumarin)
2-Chromanone
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
hydrocoumarin

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

Physical Properties

Property code	Value	Unit	Source
hf	-213.24	kJ/mol	Cheméo Relay (1.0)
hfus	15.17	kJ/mol	Joback Method
hvap	69.90 ± 0.50	kJ/mol	NIST Webbook
ie	8.56	eV	Cheméo Relay (1.0)
logp	1.538		Crippen Method
mcvol	110.490	ml/mol	McGowan Method
rinpol	1392.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1398.00		NIST Webbook

rinpol	1361.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1359.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1361.00		NIST Webbook
rinpol	1398.00		NIST Webbook
ripol	2269.00		NIST Webbook
ripol	2314.00		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
tb	545.20	K	NIST Webbook
tf	317.61	K	Cheméo Relay (1.0)

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

Experimental and computational thermochemistry of the isomers: Chromanone, 3-isochromanone, and dihydrocoumarin:	https://www.doi.org/10.1016/j.jct.2008.08.012
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119846&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point