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

Other names:	2,3-Dihydro-2-benzopyran-4-one
	2,3-Dihydro-4-benzopyranone
	2,3-dihydro-4H-1-benzopyran-4-one
	4-Chromanone
	Chroman-4-one
	Chromanone
	Isochromanone
Inchi:	InChI=1S/C9H8O2/c10-8-5-6-11-9-4-2-1-3-7(8)9/h1-4H,5-6H2
InchiKey:	MSTDXOZUKAQDRL-UHFFFAOYSA-N
Formula:	C9H8O2
SMILES:	O=C1CCOc2ccccc21
Mol. weight [g/mol]:	148.16
CAS:	491-37-2

Physical Properties

Property code	Value	Unit	Source
gf	-24.67	kJ/mol	Joback Method
hf	-186.75	kJ/mol	Joback Method
hfus	16.72	kJ/mol	Experimental and computational thermochemistry of the isomers: Chromanone, 3-isochromanone, and dihydrocoumarin
hsub	84.60 ± 1.30	kJ/mol	NIST Webbook
hvap	47.72	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	1.652		Crippen Method
mcvol	110.490	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	1390.00		NIST Webbook
ripol	2450.00		NIST Webbook
ripol	2442.00		NIST Webbook
tb	547.43	K	Joback Method
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	311.73	J/mol×K	757.10	Joback Method
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	321.13	J/mol×K	799.04	Joback Method
hfust	16.70	kJ/mol	312.30	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.20	K	1.70	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C491372&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature

hsub:	Enthalpy of sublimation 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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/44-927-4/4H-1-Benzopyran-4-one-2-3-dihydro.pdf

Generated by Cheméo on 2024-10-12 08:11:28.411662046 +0000 UTC m=+3301551.048631298.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.