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

Other names: 1,4-dihydro-3H-2-benzopyran-3-one
3-Isochromanone
Inchi: InChI=1S/C9H8O2/c10-9-5-7-3-1-2-4-8(7)6-11-9/h1-4H,5-6H2
InchiKey: ILHLUZUMRJQEAH-UHFFFAOYSA-N
Formula: C9H8O2
SMILES: O=C1Cc2ccccc2CO1
Mol. weight [g/mol]: 148.16
CAS: 4385-35-7

Physical Properties

Property code	Value	Unit	Source
gf	-24.67	kJ/mol	Joback Method
hf	-186.75	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Experimental and computational thermochemistry of the isomers: Chromanone, 3-isochromanone, and dihydrocoumarin
hsub	97.30 ± 1.40	kJ/mol	NIST Webbook
hvap	47.72	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.286		Crippen Method
mcvol	110.490	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
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	18.30	kJ/mol	355.90	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4385357&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume