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

Other names:	Chroman
	3,4-Dihydro-2H-1-benzopyran
	Benzopyran, 3,4-dihydro
	Dihydrobenzopyran
Inchi:	InChI=1S/C9H10O/c1-2-6-9-8(4-1)5-3-7-10-9/h1-2,4,6H,3,5,7H2
InchiKey:	VZWXIQHBIQLMPN-UHFFFAOYSA-N
Formula:	C9H10O
SMILES:	c1ccc2c(c1)CCCO2
Mol. weight [g/mol]:	134.18
CAS:	493-08-3

Physical Properties

Property code	Value	Unit	Source
chl	-4831.63 ± 0.92	kJ/mol	NIST Webbook
gf	97.92	kJ/mol	Joback Method
hf	-82.40 ± 1.20	kJ/mol	NIST Webbook
hfl	-139.10 ± 1.20	kJ/mol	NIST Webbook
hfus	15.66	kJ/mol	Joback Method
hsub	56.70 ± 0.10	kJ/mol	NIST Webbook
hvap	56.70	kJ/mol	NIST Webbook
hvap	56.70	kJ/mol	NIST Webbook
ie	7.93	eV	NIST Webbook
ie	8.43	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	2.012		Crippen Method
mcvol	108.920	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
sl	246.03	J/mol×K	NIST Webbook
sl	246.02	J/mol×K	NIST Webbook
tb	479.61	K	Joback Method
tc	714.33	K	Joback Method
tf	269.84	K	NIST Webbook
vc	0.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.31	J/mol×K	557.85	Joback Method
cpg	227.70	J/mol×K	479.61	Joback Method
cpg	242.55	J/mol×K	518.73	Joback Method
cpg	301.77	J/mol×K	714.33	Joback Method
cpg	291.71	J/mol×K	675.21	Joback Method
cpg	280.82	J/mol×K	636.09	Joback Method
cpg	269.05	J/mol×K	596.97	Joback Method
cpl	213.97	J/mol×K	298.15	NIST Webbook
cpl	214.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0010990	Pa×s	343.44	Joback Method
dvisc	0.0007787	Pa×s	377.49	Joback Method
dvisc	0.0005841	Pa×s	411.53	Joback Method
dvisc	0.0004578	Pa×s	445.57	Joback Method
dvisc	0.0003715	Pa×s	479.61	Joback Method
dvisc	0.0028266	Pa×s	275.36	Joback Method
dvisc	0.0016733	Pa×s	309.40	Joback Method
hfust	16.26	kJ/mol	269.84	NIST Webbook
hfust	16.26	kJ/mol	269.80	NIST Webbook
hfust	16.26	kJ/mol	269.80	NIST Webbook
hsubt	55.20 ± 0.10	kJ/mol	414.00	NIST Webbook
hsubt	42.50 ± 0.50	kJ/mol	414.00	NIST Webbook
hsubt	45.10 ± 0.30	kJ/mol	414.00	NIST Webbook
hsubt	48.90 ± 0.10	kJ/mol	414.00	NIST Webbook
hsubt	50.20 ± 0.10	kJ/mol	414.00	NIST Webbook
hsubt	52.70 ± 0.10	kJ/mol	414.00	NIST Webbook
sfust	60.24	J/mol×K	269.84	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	487.70	K	98.90	NIST Webbook
tbrp	371.70	K	2.40	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C493083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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