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

Other names: Isothiochroman
Thioisochroman
3,4-Dihydro-1H-2-benzothiopyran
Inchi: InChI=1S/C9H10S/c1-2-4-9-7-10-6-5-8(9)3-1/h1-4H,5-7H2
InchiKey: ZZQUQFZVCJWSER-UHFFFAOYSA-N
Formula: C9H10S
SMILES: c1ccc2c(c1)CCSC2
Mol. weight [g/mol]: 150.24
CAS: 4426-75-9

Physical Properties

Property code	Value	Unit	Source
gf	223.90	kJ/mol	Joback Method
hf	128.21	kJ/mol	Joback Method
hfus	11.34	kJ/mol	Joback Method
hvap	44.77	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.476		Crippen Method
mcvol	119.400	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
tb	500.49	K	Joback Method
tc	752.24	K	Joback Method
tf	332.24	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.01	J/mol×K	500.49	Joback Method
cpg	258.17	J/mol×K	542.45	Joback Method
cpg	272.10	J/mol×K	584.41	Joback Method
cpg	284.90	J/mol×K	626.37	Joback Method
cpg	296.65	J/mol×K	668.33	Joback Method

cpg	307.45	J/mol×K	710.28	Joback Method
cpg	317.39	J/mol×K	752.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4426759&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
ie:	Ionization energy
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