

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

Other names:	Thiochroman-4-one
Inchi:	InChI=1S/C9H8OS/c10-8-5-6-11-9-4-2-1-3-7(8)9/h1-4H,5-6H2
InchiKey:	CVQSWZMJOGOPAV-UHFFFAOYSA-N
Formula:	C9H8OS
SMILES:	O=C1CCSc2ccccc21
Mol. weight [g/mol]:	164.22
CAS:	3528-17-4

Physical Properties

Property code	Value	Unit	Source
gf	101.31	kJ/mol	Joback Method
hf	-9.49	kJ/mol	Joback Method
hfus	10.85	kJ/mol	Joback Method
hvap	49.02	kJ/mol	Joback Method
ie	8.53	eV	NIST Webbook
log10ws	-2.77		Crippen Method
logp	2.365		Crippen Method
mcvol	120.970	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
tb	568.31	K	Joback Method
tc	836.59	K	Joback Method
tf	400.46	K	Joback Method
vc	0.434	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.74	J/molxK	568.31	Joback Method
cpg	279.87	J/molxK	613.02	Joback Method
cpg	292.92	J/molxK	657.74	Joback Method
cpg	304.95	J/molxK	702.45	Joback Method
cpg	315.99	J/molxK	747.17	Joback Method
cpg	326.11	J/molxK	791.88	Joback Method
cpg	335.35	J/molxK	836.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.20	K	1.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3528174&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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