Benzo[b]thiophene, 2,3-dihydro-

Other names:	Benzothiophane
	1-Thiaindan
	2,3-Dihydrobenzothiophene
	2,3-Dihydrobenzo[b]thiophene
	Dihydrobenzothiophene
Inchi:	InChI=1S/C8H8S/c1-2-4-8-7(3-1)5-6-9-8/h1-4H,5-6H2
InchiKey:	YJUFGFXVASPYFQ-UHFFFAOYSA-N
Formula:	C8H8S
SMILES:	c1ccc2c(c1)CCS2
Mol. weight [g/mol]:	136.21
CAS:	4565-32-6

Physical Properties

Property code	Value	Unit	Source
gf	227.58	kJ/mol	Joback Method
hf	155.01	kJ/mol	Joback Method
hfus	10.85	kJ/mol	Joback Method
hvap	59.10 ± 0.20	kJ/mol	NIST Webbook
log10ws	-2.49		Crippen Method
logp	2.335		Crippen Method
mcvol	105.310	ml/mol	McGowan Method
pc	4368.40	kPa	Joback Method
tb	473.34	K	Joback Method
tc	719.97	K	Joback Method
tf	324.49	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.81	J/mol×K	473.34	Joback Method
cpg	256.83	J/mol×K	678.86	Joback Method
cpg	247.68	J/mol×K	637.76	Joback Method
cpg	237.69	J/mol×K	596.65	Joback Method

cpg	226.78	J/mol×K	555.55	Joback Method
cpg	214.85	J/mol×K	514.44	Joback Method
cpg	265.23	J/mol×K	719.97	Joback Method
hfust	14.84	kJ/mol	269.80	NIST Webbook
hvapt	46.40 ± 0.30	kJ/mol	451.00	NIST Webbook
hvapt	49.00 ± 0.20	kJ/mol	451.00	NIST Webbook
hvapt	51.40 ± 0.20	kJ/mol	451.00	NIST Webbook
hvapt	53.80 ± 0.20	kJ/mol	451.00	NIST Webbook
hvapt	56.30 ± 0.20	kJ/mol	451.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4565326&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
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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