Benzo[c]thiophene, 1,3,3a,4,7,7a-hexahydro-

Other names: 8-Thiabicyclo[4.3.0]non-3-ene
Inchi: InChI=1S/C8H12S/c1-2-4-8-6-9-5-7(8)3-1/h1-2,7-8H,3-6H2
InchiKey: ASTZLIXTXJMRFI-UHFFFAOYSA-N
Formula: C8H12S
SMILES: C1=CCC2CSCC2C1
Mol. weight [g/mol]: 140.25
CAS: 74601-20-0

Physical Properties

Property code	Value	Unit	Source
gf	171.50	kJ/mol	Joback Method
hf	21.71	kJ/mol	Joback Method
hfus	11.32	kJ/mol	Joback Method
hvap	39.85	kJ/mol	Joback Method
ie	8.22	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.316		Crippen Method
mcvol	113.910	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
tb	455.72	K	Joback Method
tc	693.67	K	Joback Method
tf	289.45	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.16	J/mol×K	455.72	Joback Method
cpg	251.07	J/mol×K	495.38	Joback Method
cpg	267.68	J/mol×K	535.04	Joback Method
cpg	283.07	J/mol×K	574.70	Joback Method
cpg	297.31	J/mol×K	614.36	Joback Method
cpg	310.49	J/mol×K	654.01	Joback Method

cpg	322.68	J/mol×K	693.67	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74601200&Units=SI

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