

Benzo[c]thiophene, 1,3-dihydro-

Other names:	o-Xylylene sulfide 1,3-Dihydrobenzo[c]thiophene Dihydrobenzo(c)thiophene
Inchi:	InChI=1S/C8H8S/c1-2-4-8-6-9-5-7(8)3-1/h1-4H,5-6H2
InchiKey:	KVRZARWOKBNZMM-UHFFFAOYSA-N
Formula:	C8H8S
SMILES:	c1ccc2c(c1)CSC2
Mol. weight [g/mol]:	136.21
CAS:	2471-92-3

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	42.37	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.51	eV	NIST Webbook
log10ws	-3.01		Crippen Method
logp	2.433		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	214.85	J/mol×K	514.44	Joback Method
cpg	226.78	J/mol×K	555.55	Joback Method
cpg	237.69	J/mol×K	596.65	Joback Method

cpg	247.68	J/mol×K	637.76	Joback Method
cpg	256.83	J/mol×K	678.86	Joback Method
cpg	265.23	J/mol×K	719.97	Joback Method

Sources

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=C2471923&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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