Benzene, (ethylthio)-

Other names:	Sulfide, ethyl phenyl (Ethylthio)benzene (Phenylthio)ethane Ethyl phenyl sulfide Phenyl ethyl sulfide Thiophenetole Ethyl phenyl sulphide (1-Thiapropyl)benzene NSC 75124
Inchi:	InChI=1S/C8H10S/c1-2-9-8-6-4-3-5-7-8/h3-7H,2H2,1H3
InchiKey:	AEHWKBXBXYNPCX-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	CCSc1ccccc1
Mol. weight [g/mol]:	138.23
CAS:	622-38-8

Physical Properties

Property code	Value	Unit	Source
chl	-5201.00 ± 1.50	kJ/mol	NIST Webbook
gf	162.01	kJ/mol	Joback Method
hf	77.00 ± 3.00	kJ/mol	NIST Webbook
hfl	21.90 ± 1.50	kJ/mol	NIST Webbook
hfus	14.65	kJ/mol	Joback Method
hvap	55.10	kJ/mol	NIST Webbook
hvap	56.40	kJ/mol	NIST Webbook
hvap	55.00 ± 2.00	kJ/mol	NIST Webbook
ie	7.88 ± 0.02	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.53	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-2.63		Crippen Method
logp	2.799		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
rinpol	1160.00		NIST Webbook
rinpol	1160.00		NIST Webbook
tb	478.20	K	NIST Webbook

tc	712.59	K	Joback Method
tf	240.74	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.99	J/mol×K	477.90	Joback Method
cpg	236.28	J/mol×K	517.01	Joback Method
cpg	248.73	J/mol×K	556.13	Joback Method
cpg	260.36	J/mol×K	595.24	Joback Method
cpg	271.21	J/mol×K	634.36	Joback Method
cpg	281.31	J/mol×K	673.47	Joback Method
cpg	290.68	J/mol×K	712.59	Joback Method
hvapt	50.90	kJ/mol	352.50	NIST Webbook
hvapt	51.70	kJ/mol	407.50	NIST Webbook
hvapt	53.60 ± 2.10	kJ/mol	340.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C622388&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

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume