Benzene, 1-(ethylthio)-3-methyl-

Inchi: InChI=1S/C9H12S/c1-3-10-9-6-4-5-8(2)7-9/h4-7H,3H2,1-2H3
InchiKey: HYWRFKLTGRADFO-UHFFFAOYSA-N
Formula: C9H12S
SMILES: CCSc1cccc(C)c1
Mol. weight [g/mol]: 152.26
CAS: 34786-24-8

Physical Properties

Property code	Value	Unit	Source
gf	160.80	kJ/mol	Joback Method
hf	37.84	kJ/mol	Joback Method
hfus	16.85	kJ/mol	Joback Method
hvap	45.38	kJ/mol	Joback Method
ie	7.92	eV	NIST Webbook
log10ws	-3.11		Crippen Method
logp	3.107		Crippen Method
mcvol	130.260	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
tb	505.76	K	Joback Method
tc	737.59	K	Joback Method
tf	264.53	K	Joback Method
vc	0.485	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.45	J/mol×K	698.95	Joback Method
cpg	265.45	J/mol×K	505.76	Joback Method
cpg	279.46	J/mol×K	544.40	Joback Method
cpg	292.64	J/mol×K	583.04	Joback Method
cpg	305.01	J/mol×K	621.68	Joback Method
cpg	316.61	J/mol×K	660.32	Joback Method
cpg	337.56	J/mol×K	737.59	Joback Method
hvapt	43.50	kJ/mol	487.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34786248&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume