Phenol, 2-[(ethylthio)methyl]-

Other names:	Ethyl 2-hydroxybenzyl sulfide
	«alpha»-(ethylthio)-o-cresol
Inchi:	InChI=1S/C9H12OS/c1-2-11-7-8-5-3-4-6-9(8)10/h3-6,10H,2,7H2,1H3
InchiKey:	QZBBPVLBIUUYRH-UHFFFAOYSA-N
Formula:	C9H12OS
SMILES:	CCSCc1ccccc1O
Mol. weight [g/mol]:	168.26
CAS:	65370-06-1

Physical Properties

Property code	Value	Unit	Source
gf	15.81	kJ/mol	Joback Method
hf	-128.00	kJ/mol	Joback Method
hfus	23.02	kJ/mol	Joback Method
hvap	57.73	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.645		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
rinpol	1404.00		NIST Webbook
tb	581.40	K	Joback Method
tc	823.84	K	Joback Method
tf	363.73	K	Joback Method
vc	0.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.08	J/mol×K	581.40	Joback Method
cpg	327.90	J/mol×K	621.81	Joback Method
cpg	339.77	J/mol×K	662.21	Joback Method
cpg	350.79	J/mol×K	702.62	Joback Method
cpg	361.04	J/mol×K	743.03	Joback Method
cpg	370.61	J/mol×K	783.44	Joback Method

cpg	379.60	J/mol×K	823.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65370061&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
hvap:	Enthalpy of vaporization at standard conditions
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