Ethyl 2-hydroxybenzyl sulfide

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

Physical Properties

Property code	Value	Unit	Source
hf	-117.54	kJ/mol	Cheméo Relay (1.0)
hfus	23.02	kJ/mol	Joback Method
hvap	75.19	kJ/mol	Cheméo Relay (1.0)
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-1.46		Cheméo Relay (1.0)
logp	2.645		Crippen Method
mcvol	136.130	ml/mol	McGowan Method
rinpol	1404.00		NIST Webbook
tb	547.53	K	Cheméo Relay (1.0)
tc	774.20	K	Cheméo Relay (1.0)
tf	312.49	K	Cheméo Relay (1.0)

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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point