

4-Ethylthiophenol

Other names:	4-Ethylbenzenethiol
Inchi:	InChI=1S/C8H10S/c1-2-7-3-5-8(9)6-4-7/h3-6,9H,2H2,1H3
InchiKey:	WWQQPHUHTAZWDH-UHFFFAOYSA-N
Formula:	C8H10S
SMILES:	CCc1ccc(S)cc1
Mol. weight [g/mol]:	138.23
CAS:	4946-13-8

Physical Properties

Property code	Value	Unit	Source
gf	148.65	kJ/mol	Joback Method
hf	55.09	kJ/mol	Joback Method
hfus	14.17	kJ/mol	Joback Method
hvap	43.08	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.538		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
pc	3877.12	kPa	Joback Method
tb	476.96	K	Joback Method
tc	713.39	K	Joback Method
tf	255.32	K	Joback Method
vc	0.429	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.48	J/mol×K	476.96	Joback Method
cpg	234.25	J/mol×K	516.37	Joback Method
cpg	246.23	J/mol×K	555.77	Joback Method
cpg	257.43	J/mol×K	595.18	Joback Method
cpg	267.90	J/mol×K	634.58	Joback Method
cpg	277.66	J/mol×K	673.99	Joback Method
cpg	286.76	J/mol×K	713.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4946138&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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