

4-ETHOXYMETHYLPHENOL

Other names:	4-Ethoxymethylphenol «alpha»-ethoxy-p-cresol
Inchi:	InChI=1S/C9H12O2/c1-2-11-7-8-3-5-9(10)6-4-8/h3-6,10H,2,7H2,1H3
InchiKey:	UWQZVUQKBWZNLN-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CCOCc1ccc(O)cc1
Mol. weight [g/mol]:	152.19

Physical Properties

Property code	Value	Unit	Source
hf	-275.09	kJ/mol	Cheméo Relay (1.0)
hfus	20.08	kJ/mol	Joback Method
hvap	70.98	kJ/mol	Cheméo Relay (1.0)
ie	8.26	eV	Cheméo Relay (1.0)
log10ws	-0.96		Cheméo Relay (1.0)
logp	1.929		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
tb	520.94	K	Cheméo Relay (1.0)
tc	728.82	K	Cheméo Relay (1.0)
tf	319.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.27	J/mol×K	535.04	Joback Method
cpg	302.86	J/mol×K	571.65	Joback Method
cpg	314.65	J/mol×K	608.25	Joback Method
cpg	325.69	J/mol×K	644.86	Joback Method
cpg	336.05	J/mol×K	681.47	Joback Method
cpg	345.78	J/mol×K	718.08	Joback Method
cpg	354.94	J/mol×K	754.68	Joback Method
dvisc	0.0022554	Pa×s	351.56	Joback Method
dvisc	0.0009440	Pa×s	382.14	Joback Method
dvisc	0.0004496	Pa×s	412.72	Joback Method

dvisc	0.0002372	Pa×s	443.30	Joback Method
dvisc	0.0001359	Pa×s	473.88	Joback Method
dvisc	0.0000833	Pa×s	504.46	Joback Method
dvisc	0.0000540	Pa×s	535.04	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57726268&Units=SI
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
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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