Phenol, 4-(ethoxymethyl)-2-methoxy-

Other names:	4-(Ethoxymethyl)-2-methoxyphenol
	Ethyl vanillyl ether
	Vanillyl ethyl ether
	Ethyl 4-hydroxy-3-methoxybenzyl ether
Inchi:	InChI=1S/C10H14O3/c1-3-13-7-8-4-5-9(11)10(6-8)12-2/h4-6,11H,3,7H2,1-2H3
InchiKey:	KOCVACNWDMSLBM-UHFFFAOYSA-N
Formula:	C10H14O3
SMILES:	CCOCc1ccc(O)c(OC)c1
Mol. weight [g/mol]:	182.22
CAS:	13184-86-6

Physical Properties

Property code	Value	Unit	Source
gf	-228.52	kJ/mol	Joback Method
hf	-466.42	kJ/mol	Joback Method
hfus	23.47	kJ/mol	Joback Method
hvap	58.63	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	1.937		Crippen Method
mcvol	145.610	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1553.00		NIST Webbook
rinpol	1466.20		NIST Webbook
rinpol	1553.00		NIST Webbook
ripol	2941.00		NIST Webbook
tb	585.32	K	Joback Method
tc	799.74	K	Joback Method
tf	397.58	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.81	J/mol×K	585.32	Joback Method

cpg	371.74	J/mol×K	621.06	Joback Method
cpg	383.98	J/mol×K	656.79	Joback Method
cpg	395.55	J/mol×K	692.53	Joback Method
cpg	406.50	J/mol×K	728.26	Joback Method
cpg	416.86	J/mol×K	764.00	Joback Method
cpg	426.67	J/mol×K	799.74	Joback Method
dvisc	0.0007101	Pa×s	397.58	Joback Method
dvisc	0.0003414	Pa×s	428.87	Joback Method
dvisc	0.0001813	Pa×s	460.16	Joback Method
dvisc	0.0001044	Pa×s	491.45	Joback Method
dvisc	0.0000642	Pa×s	522.74	Joback Method
dvisc	0.0000417	Pa×s	554.03	Joback Method
dvisc	0.0000284	Pa×s	585.32	Joback Method

Sources

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=C13184866&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume

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