PHENOL, 2-ETHOXY-4-METHYL-

Other names: Phenol, 2-ethoxy-4-methyl-
Inchi: InChI=1S/C9H12O2/c1-3-11-9-6-7(2)4-5-8(9)10/h4-6,10H,3H2,1-2H3
InchiKey: ZWQBCCVEOIYNDL-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CCOc1cc(C)ccc1O
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
hf	-321.36	kJ/mol	Cheméo Relay (1.0)
hfus	19.69	kJ/mol	Joback Method
hvap	65.37	kJ/mol	Cheméo Relay (1.0)
ie	7.82	eV	Cheméo Relay (1.0)
log10ws	-1.89		Cheméo Relay (1.0)
logp	2.099		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	509.46	K	Cheméo Relay (1.0)
tc	721.20	K	Cheméo Relay (1.0)
tf	322.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.84	J/mol×K	540.02	Joback Method
cpg	353.30	J/mol×K	760.79	Joback Method
cpg	344.22	J/mol×K	724.00	Joback Method
cpg	334.61	J/mol×K	687.20	Joback Method
cpg	324.42	J/mol×K	650.41	Joback Method
cpg	313.60	J/mol×K	613.61	Joback Method
cpg	302.09	J/mol×K	576.82	Joback Method
dvisc	0.0001968	Pa×s	452.05	Joback Method
dvisc	0.0000505	Pa×s	540.02	Joback Method
dvisc	0.0000754	Pa×s	510.70	Joback Method

dvisc	0.0001183	Pa×s	481.37	Joback Method
dvisc	0.0014803	Pa×s	364.08	Joback Method
dvisc	0.0003513	Pa×s	422.73	Joback Method
dvisc	0.0006835	Pa×s	393.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.50 ± 1.50	K	1.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2563077&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

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
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point