

2-Ethoxy-4-methylphenol

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
CAS:	2563-07-7

Physical Properties

Property code	Value	Unit	Source
gf	-131.94	kJ/mol	Joback Method
hf	-313.56	kJ/mol	Joback Method
hfus	19.69	kJ/mol	Joback Method
hvap	53.99	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.099		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	540.02	K	Joback Method
tc	760.79	K	Joback Method
tf	364.08	K	Joback Method
vc	0.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.84	J/molxK	540.02	Joback Method
cpg	302.09	J/molxK	576.82	Joback Method
cpg	313.60	J/molxK	613.61	Joback Method
cpg	324.42	J/molxK	650.41	Joback Method
cpg	334.61	J/molxK	687.20	Joback Method
cpg	344.22	J/molxK	724.00	Joback Method
cpg	353.30	J/molxK	760.79	Joback Method
dvisc	0.0014803	Paxs	364.08	Joback Method

dvisc	0.0006835	Paxs	393.40	Joback Method
dvisc	0.0003513	Paxs	422.73	Joback Method
dvisc	0.0001968	Paxs	452.05	Joback Method
dvisc	0.0001183	Paxs	481.37	Joback Method
dvisc	0.0000754	Paxs	510.70	Joback Method
dvisc	0.0000505	Paxs	540.02	Joback Method

Pressure Dependent Properties

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

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=C2563077&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

tf: Normal melting (fusion) point

vc: Critical Volume

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