

3-Ethyl-5-methoxyphenol

Inchi:	InChI=1S/C9H12O2/c1-3-7-4-8(10)6-9(5-7)11-2/h4-6,10H,3H2,1-2H3
InchiKey:	VKVVAKEARYUDV-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CCc1cc(O)cc(OC)c1
Mol. weight [g/mol]:	152.19

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	-1.94		Crippen Method
logp	1.963		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
ripol	2253.00		NIST Webbook
ripol	2253.00		NIST Webbook
tb	540.02	K	Joback Method
tc	760.79	K	Joback Method
tf	364.08	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0006835	Pa×s	393.40	Joback Method
dvisc	0.0003513	Pa×s	422.73	Joback Method
dvisc	0.0001968	Pa×s	452.05	Joback Method
dvisc	0.0001183	Pa×s	481.37	Joback Method
dvisc	0.0000754	Pa×s	510.70	Joback Method
dvisc	0.0000505	Pa×s	540.02	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=R403460&Units=SI

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

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