Ethyl guaiacol

Other names: Benzene, 1-ethoxy-2-methoxy-
2-methoxyphenetole
Inchi: InChI=1S/C9H12O2/c1-3-11-9-7-5-4-6-8(9)10-2/h4-7H,3H2,1-2H3
InchiKey: OMONCKYJLBVWOQ-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CCOc1ccccc1OC
Mol. weight [g/mol]: 152.19
CAS: 17600-72-5

Physical Properties

Property code	Value	Unit	Source
gf	-82.32	kJ/mol	Joback Method
hf	-268.47	kJ/mol	Joback Method
hfus	15.09	kJ/mol	Joback Method
hvap	43.39	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	2.094		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1280.00		NIST Webbook
tb	481.00 ± 1.00	K	NIST Webbook
tc	687.40	K	Joback Method
tf	274.59	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.58	J/mol×K	481.82	Joback Method
cpg	321.73	J/mol×K	653.13	Joback Method
cpg	310.98	J/mol×K	618.87	Joback Method
cpg	299.69	J/mol×K	584.61	Joback Method

cpg	287.86	J/mol×K	550.35	Joback Method
cpg	275.49	J/mol×K	516.08	Joback Method
cpg	331.92	J/mol×K	687.40	Joback Method
dvisc	0.0001671	Pa×s	481.82	Joback Method
dvisc	0.0002086	Pa×s	447.28	Joback Method
dvisc	0.0002703	Pa×s	412.74	Joback Method
dvisc	0.0003671	Pa×s	378.21	Joback Method
dvisc	0.0005303	Pa×s	343.67	Joback Method
dvisc	0.0008317	Pa×s	309.13	Joback Method
dvisc	0.0014607	Pa×s	274.59	Joback Method

Sources

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=C17600725&Units=SI
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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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