

Benzene, 1-ethoxy-4-methoxy-

Other names:	p-Ethoxyanisole Ethyl p-methoxyphenyl ether p-methoxyphenetole
Inchi:	InChI=1S/C9H12O2/c1-3-11-9-6-4-8(10-2)5-7-9/h4-7H,3H2,1-2H3
InchiKey:	FTFNFGIOGXKJSP-UHFFFAOYSA-N
Formula:	C9H12O2
SMILES:	CCOc1ccc(OC)cc1
Mol. weight [g/mol]:	152.19
CAS:	5076-72-2

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
ie	8.03 ± 0.15	eV	NIST Webbook
ie	7.72 ± 0.01	eV	NIST Webbook
log10ws	-2.13		Crippen Method
logp	2.094		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	481.82	K	Joback Method
tc	687.40	K	Joback Method
tf	312.00	K	NIST Webbook
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.58	J/molxK	481.82	Joback Method
cpg	275.49	J/molxK	516.08	Joback Method
cpg	287.86	J/molxK	550.35	Joback Method
cpg	299.69	J/molxK	584.61	Joback Method

cpg	310.98	J/molxK	618.87	Joback Method
cpg	321.73	J/molxK	653.13	Joback Method
cpg	331.92	J/molxK	687.40	Joback Method
dvisc	0.0014607	Paxs	274.59	Joback Method
dvisc	0.0008317	Paxs	309.13	Joback Method
dvisc	0.0005303	Paxs	343.67	Joback Method
dvisc	0.0003671	Paxs	378.21	Joback Method
dvisc	0.0002703	Paxs	412.74	Joback Method
dvisc	0.0002086	Paxs	447.28	Joback Method
dvisc	0.0001671	Paxs	481.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	489.50 ± 0.50	K	101.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5076722&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
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
vc:	Critical Volume

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