Benzene, 1-methylethoxy-

Other names: isopropoxybenzene
Inchi: InChI=1S/C9H12O/c1-8(2)10-9-6-4-3-5-7-9/h3-8H,1-2H3
InchiKey: ZYNMJJNWXVKJJV-UHFFFAOYSA-N
Formula: C9H12O
SMILES: CC(C)Oc1ccccc1
Mol. weight [g/mol]: 136.19
CAS: 2741-16-4

Physical Properties

Property code	Value	Unit	Source
gf	29.87	kJ/mol	Joback Method
hf	-130.06	kJ/mol	Joback Method
hfus	10.77	kJ/mol	Joback Method
hvap	39.93	kJ/mol	Joback Method
ie	8.32	eV	NIST Webbook
log10ws	-2.54		Crippen Method
logp	2.474		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1027.00		NIST Webbook
rinpol	1016.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	450.00 ± 0.50	K	NIST Webbook
tb	450.40 ± 0.50	K	NIST Webbook
tc	664.69	K	Joback Method
tf	240.10 ± 0.30	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.41	J/mol×K	664.69	Joback Method
cpg	301.80	J/mol×K	629.57	Joback Method

cpg	290.55	J/mol×K	594.45	Joback Method
cpg	278.62	J/mol×K	559.33	Joback Method
cpg	266.01	J/mol×K	524.22	Joback Method
cpg	252.69	J/mol×K	489.10	Joback Method
cpg	238.66	J/mol×K	453.98	Joback Method
dvisc	0.0040329	Pa×s	224.84	Joback Method
dvisc	0.0001942	Pa×s	453.98	Joback Method
dvisc	0.0002553	Pa×s	415.79	Joback Method
dvisc	0.0003546	Pa×s	377.60	Joback Method
dvisc	0.0005304	Pa×s	339.41	Joback Method
dvisc	0.0008786	Pa×s	301.22	Joback Method
dvisc	0.0016853	Pa×s	263.03	Joback Method
hvapt	49.50	kJ/mol	396.50	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=C2741164&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
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
ripol: Polar retention indices

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