Benzene, 1-(1,1-dimethylethyl)-4-methoxy-

Other names: Anisole, p-tert-butyl-
p-tert-Butylanisole
p-Methoxy-tert-butylbenzene
4-tert-Butylanisole
Benzene, 1-methoxy-4-t-butyl
4-tert-Butylphenyl methyl ether
Inchi: InChI=1S/C11H16O/c1-11(2,3)9-5-7-10(12-4)8-6-9/h5-8H,1-4H3
InchiKey: MCUPBIBNSTXCPQ-UHFFFAOYSA-N
Formula: C11H16O
SMILES: COc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 164.24
CAS: 5396-38-3

Physical Properties

Property code	Value	Unit	Source
gf	42.36	kJ/mol	Joback Method
hf	-186.28	kJ/mol	Joback Method
hfus	11.67	kJ/mol	Joback Method
hvap	44.13	kJ/mol	Joback Method
ie	7.77 ± 0.02	eV	NIST Webbook
log10ws	-2.90		Crippen Method
logp	2.993		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1218.00		NIST Webbook
tb	496.40 ± 0.50	K	NIST Webbook
tc	716.64	K	Joback Method
tf	292.29 ± 0.20	K	NIST Webbook
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.05	J/mol×K	501.93	Joback Method

cpg	402.27	J/mol×K	680.86	Joback Method
cpg	389.41	J/mol×K	645.07	Joback Method
cpg	375.70	J/mol×K	609.29	Joback Method
cpg	361.09	J/mol×K	573.50	Joback Method
cpg	345.56	J/mol×K	537.72	Joback Method
cpg	414.31	J/mol×K	716.64	Joback Method
dvisc	0.0001715	Pa×s	501.93	Joback Method
dvisc	0.0002251	Pa×s	464.50	Joback Method
dvisc	0.0003097	Pa×s	427.06	Joback Method
dvisc	0.0004530	Pa×s	389.62	Joback Method
dvisc	0.0007186	Pa×s	352.19	Joback Method
dvisc	0.0012719	Pa×s	314.75	Joback Method
dvisc	0.0026267	Pa×s	277.32	Joback Method

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=C5396383&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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume