

Benzene, 1-(1,1-dimethylethoxy)-2-methyl-

Other names:	Ether, tert-butyl o-tolyl
Inchi:	InChI=1S/C11H16O/c1-9-7-5-6-8-10(9)12-11(2,3)4/h5-8H,1-4H3
InchiKey:	LSMDIYCJNRNBA-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	<chem>Cc1ccccc1OC(C)(C)C</chem>
Mol. weight [g/mol]:	164.24
CAS:	15359-96-3

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	8.45	eV	NIST Webbook
log10ws	-3.43		Crippen Method
logp	3.172		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
tb	501.93	K	Joback Method
tc	716.64	K	Joback Method
tf	277.32	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.05	J/molxK	501.93	Joback Method
cpg	345.56	J/molxK	537.72	Joback Method
cpg	361.09	J/molxK	573.50	Joback Method
cpg	375.70	J/molxK	609.29	Joback Method
cpg	389.41	J/molxK	645.07	Joback Method
cpg	402.27	J/molxK	680.86	Joback Method
cpg	414.31	J/molxK	716.64	Joback Method

dvisc	0.0026267	Paxs	277.32	Joback Method
dvisc	0.0012719	Paxs	314.75	Joback Method
dvisc	0.0007186	Paxs	352.19	Joback Method
dvisc	0.0004530	Paxs	389.62	Joback Method
dvisc	0.0003097	Paxs	427.06	Joback Method
dvisc	0.0002251	Paxs	464.50	Joback Method
dvisc	0.0001715	Paxs	501.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15359963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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