(3-Methoxyphenyl) methanol, tert.-butyl ether

Inchi: InChI=1S/C12H18O2/c1-12(2,3)14-9-10-6-5-7-11(8-10)13-4/h5-8H,9H2,1-4H3
InchiKey: WWSILOPDQGQAJM-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: COc1cccc(COC(C)(C)C)c1
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-54.22	kJ/mol	Joback Method
hf	-339.14	kJ/mol	Joback Method
hfus	15.45	kJ/mol	Joback Method
hvap	48.77	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.010		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2336.03	kPa	Joback Method
rinpol	1427.00		NIST Webbook
tb	547.23	K	Joback Method
tc	756.39	K	Joback Method
tf	310.82	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.69	J/mol×K	547.23	Joback Method
cpg	476.78	J/mol×K	721.53	Joback Method
cpg	463.50	J/mol×K	686.67	Joback Method
cpg	449.38	J/mol×K	651.81	Joback Method
cpg	434.39	J/mol×K	616.95	Joback Method
cpg	418.50	J/mol×K	582.09	Joback Method
cpg	489.24	J/mol×K	756.39	Joback Method
dvisc	0.0001270	Pa×s	547.23	Joback Method
dvisc	0.0001664	Pa×s	507.83	Joback Method

dvisc	0.0002282	Pa×s	468.43	Joback Method
dvisc	0.0003317	Pa×s	429.02	Joback Method
dvisc	0.0005200	Pa×s	389.62	Joback Method
dvisc	0.0009020	Pa×s	350.22	Joback Method
dvisc	0.0017989	Pa×s	310.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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