

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

Inchi:	InChI=1S/C12H18O/c1-10-6-5-7-11(8-10)9-13-12(2,3)4/h5-8H,9H2,1-4H3
InchiKey:	WIAUQNWVCMSSYG-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	Cc1cccc(COC(C)(C)C)c1
Mol. weight [g/mol]:	178.27

Physical Properties

Property code	Value	Unit	Source
gf	50.78	kJ/mol	Joback Method
hf	-206.92	kJ/mol	Joback Method
hfus	14.26	kJ/mol	Joback Method
hvap	46.36	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.310		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2374.90	kPa	Joback Method
rinsol	1282.00		NIST Webbook
tb	524.81	K	Joback Method
tc	736.13	K	Joback Method
tf	288.59	K	Joback Method
vc	0.607	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.40	J/mol×K	524.81	Joback Method
cpg	392.68	J/mol×K	560.03	Joback Method
cpg	408.95	J/mol×K	595.25	Joback Method
cpg	424.27	J/mol×K	630.47	Joback Method
cpg	438.66	J/mol×K	665.69	Joback Method
cpg	452.17	J/mol×K	700.91	Joback Method
cpg	464.83	J/mol×K	736.13	Joback Method
dvisc	0.0025519	Paxs	288.59	Joback Method
dvisc	0.0012144	Paxs	327.96	Joback Method

dvisc	0.0006777	Paxs	367.33	Joback Method
dvisc	0.0004233	Paxs	406.70	Joback Method
dvisc	0.0002874	Paxs	446.07	Joback Method
dvisc	0.0002077	Paxs	485.44	Joback Method
dvisc	0.0001576	Paxs	524.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374587&Units=SI

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

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