2-Methyl-6-t-butylanisole

Inchi: InChI=1S/C12H18O/c1-9-7-6-8-10(11(9)13-5)12(2,3)4/h6-8H,1-5H3
InchiKey: XLPWABAEWSNQJE-UHFFFAOYSA-N
Formula: C12H18O
SMILES: COc1c(C)cccc1C(C)(C)C
Mol. weight [g/mol]: 178.27
CAS: 60772-80-7

Physical Properties

Property code	Value	Unit	Source
gf	41.15	kJ/mol	Joback Method
hf	-218.39	kJ/mol	Joback Method
hfus	13.87	kJ/mol	Joback Method
hvap	47.02	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.301		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	529.79	K	Joback Method
tc	742.25	K	Joback Method
tf	301.11	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	375.81	J/mol×K	529.79	Joback Method
cpg	392.73	J/mol×K	565.20	Joback Method
cpg	408.71	J/mol×K	600.61	Joback Method
cpg	423.77	J/mol×K	636.02	Joback Method
cpg	437.96	J/mol×K	671.43	Joback Method
cpg	451.31	J/mol×K	706.84	Joback Method
cpg	463.85	J/mol×K	742.25	Joback Method
dvisc	0.0018283	Pa×s	301.11	Joback Method
dvisc	0.0009574	Pa×s	339.22	Joback Method

dvisc	0.0005713	Pa×s	377.34	Joback Method
dvisc	0.0003748	Pa×s	415.45	Joback Method
dvisc	0.0002639	Pa×s	453.56	Joback Method
dvisc	0.0001962	Pa×s	491.68	Joback Method
dvisc	0.0001523	Pa×s	529.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60772807&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
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
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