o-(tert-Butyl)anisole

Inchi: InChI=1S/C11H16O/c1-11(2,3)9-7-5-6-8-10(9)12-4/h5-8H,1-4H3
InchiKey: YIQUTYFGUKCQCY-UHFFFAOYSA-N
Formula: C11H16O
SMILES: COc1ccccc1C(C)(C)C
Mol. weight [g/mol]: 164.24

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
log10ws	-2.90		Crippen Method
logp	2.993		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2613.74	kPa	Joback Method
rinpol	1170.00		NIST Webbook
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/mol×K	501.93	Joback Method
cpg	345.56	J/mol×K	537.72	Joback Method
cpg	361.09	J/mol×K	573.50	Joback Method
cpg	375.70	J/mol×K	609.29	Joback Method
cpg	389.41	J/mol×K	645.07	Joback Method
cpg	402.27	J/mol×K	680.86	Joback Method
cpg	414.31	J/mol×K	716.64	Joback Method
dvisc	0.0026267	Pa×s	277.32	Joback Method
dvisc	0.0012719	Pa×s	314.75	Joback Method

dvisc	0.0007186	Pa×s	352.19	Joback Method
dvisc	0.0004530	Pa×s	389.62	Joback Method
dvisc	0.0003097	Pa×s	427.06	Joback Method
dvisc	0.0002251	Pa×s	464.50	Joback Method
dvisc	0.0001715	Pa×s	501.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R543607&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