o-(sec-Butyl)anisole

Inchi: InChI=1S/C11H16O/c1-4-9(2)10-7-5-6-8-11(10)12-3/h5-9H,4H2,1-3H3
InchiKey: XGEOZYQKQHPUFZ-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CCC(C)c1ccccc1OC
Mol. weight [g/mol]: 164.24

Physical Properties

Property code	Value	Unit	Source
gf	37.08	kJ/mol	Joback Method
hf	-182.81	kJ/mol	Joback Method
hfus	15.56	kJ/mol	Joback Method
hvap	45.04	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.209		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	504.72	K	Joback Method
tc	710.80	K	Joback Method
tf	259.90	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.28	J/mol×K	504.72	Joback Method
cpg	341.96	J/mol×K	539.07	Joback Method
cpg	356.87	J/mol×K	573.41	Joback Method
cpg	371.02	J/mol×K	607.76	Joback Method
cpg	384.44	J/mol×K	642.11	Joback Method
cpg	397.14	J/mol×K	676.45	Joback Method
cpg	409.13	J/mol×K	710.80	Joback Method
dvisc	0.0027032	Pa×s	259.90	Joback Method

dvisc	0.0012429	Pa×s	300.70	Joback Method
dvisc	0.0006880	Pa×s	341.51	Joback Method
dvisc	0.0004321	Pa×s	382.31	Joback Method
dvisc	0.0002969	Pa×s	423.11	Joback Method
dvisc	0.0002179	Pa×s	463.92	Joback Method
dvisc	0.0001681	Pa×s	504.72	Joback Method

Sources

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=R543598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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