4-Methylphenol, n-butyl ether

Other names:	n-Butyl p-tolyl ether
	4-(n-Butoxy)toluene
	Benzene, 1-butoxy-4-methyl-
	butyl p-tolyl ether
Inchi:	InChI=1S/C11H16O/c1-3-4-9-12-11-7-5-10(2)6-8-11/h5-8H,3-4,9H2,1-2H3
InchiKey:	AGARRLZBNOJWLG-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	CCCCOc1ccc(C)cc1
Mol. weight [g/mol]:	164.25

Physical Properties

Property code	Value	Unit	Source
af	0.5192		Cheméo Relay (1.0)
gf	39.52	kJ/mol	Joback Method
hf	-182.10	kJ/mol	Cheméo Relay (1.0)
hfus	19.09	kJ/mol	Joback Method
hvap	56.34	kJ/mol	Cheméo Relay (1.0)
ie	7.92	eV	Cheméo Relay (1.0)
log10ws	-3.66		Cheméo Relay (1.0)
logp	3.174		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2563.69	kPa	Joback Method
tb	497.39	K	Cheméo Relay (1.0)
tc	694.79	K	Cheméo Relay (1.0)
tf	259.02	K	Cheméo Relay (1.0)
vc	0.554	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.06	J/mol×K	505.16	Joback Method
cpg	341.32	J/mol×K	538.75	Joback Method
cpg	355.85	J/mol×K	572.35	Joback Method
cpg	369.68	J/mol×K	605.94	Joback Method

cpg	382.80	J/mol×K	639.54	Joback Method
cpg	395.24	J/mol×K	673.13	Joback Method
cpg	407.02	J/mol×K	706.73	Joback Method
dvisc	0.0019708	Pa×s	274.90	Joback Method
dvisc	0.0010326	Pa×s	313.28	Joback Method
dvisc	0.0006230	Pa×s	351.65	Joback Method
dvisc	0.0004152	Pa×s	390.03	Joback Method
dvisc	0.0002975	Pa×s	428.41	Joback Method
dvisc	0.0002253	Pa×s	466.78	Joback Method
dvisc	0.0001779	Pa×s	505.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.00 ± 1.00	K	2.30	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10519069&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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

ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume