4-Bromophenol, n-butyl ether

Inchi: InChI=1S/C10H13BrO/c1-2-3-8-12-10-6-4-9(11)5-7-10/h4-7H,2-3,8H2,1H3
InchiKey: BOUVKHWPQNEXTO-UHFFFAOYSA-N
Formula: C10H13BrO
SMILES: CCCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 229.12

Physical Properties

Property code	Value	Unit	Source
hfus	21.78	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Cheméo Relay (1.0)
ie	8.16	eV	Cheméo Relay (1.0)
log10ws	-4.45		Cheméo Relay (1.0)
logp	3.628		Crippen Method
mcvol	151.370	ml/mol	McGowan Method
tb	530.48	K	Cheméo Relay (1.0)
tf	275.15	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.07	J/mol×K	548.44	Joback Method
cpg	335.63	J/mol×K	585.00	Joback Method
cpg	348.41	J/mol×K	621.57	Joback Method
cpg	360.44	J/mol×K	658.13	Joback Method
cpg	371.74	J/mol×K	694.70	Joback Method
cpg	382.35	J/mol×K	731.26	Joback Method
cpg	392.28	J/mol×K	767.82	Joback Method
dvisc	0.0016322	Pa×s	323.43	Joback Method
dvisc	0.0009634	Pa×s	360.93	Joback Method
dvisc	0.0006280	Pa×s	398.43	Joback Method
dvisc	0.0004406	Pa×s	435.94	Joback Method
dvisc	0.0003270	Pa×s	473.44	Joback Method
dvisc	0.0002536	Pa×s	510.94	Joback Method
dvisc	0.0002036	Pa×s	548.44	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	419.50 ± 1.50	K	6.70	NIST Webbook

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39969578&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point