3-Butylphenol

Other names: Phenol, 3-butyl-
Inchi: InChI=1S/C10H14O/c1-2-3-5-9-6-4-7-10(11)8-9/h4,6-8,11H,2-3,5H2,1H3
InchiKey: MQSXUKPGWMJYBT-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CCCCc1cccc(O)c1
Mol. weight [g/mol]: 150.22
CAS: 4074-43-5

Physical Properties

Property code	Value	Unit	Source
gf	-8.89	kJ/mol	Joback Method
hf	-190.51	kJ/mol	Joback Method
hfus	21.48	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
ie	8.90 ± 0.10	eV	NIST Webbook
log10ws	-2.66		Crippen Method
logp	2.735		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1302.00		NIST Webbook
rinpol	1302.00		NIST Webbook
tb	521.15 ± 3.00	K	NIST Webbook
tb	521.20	K	NIST Webbook
tb	521.15 ± 2.00	K	NIST Webbook
tb	521.15 ± 3.00	K	NIST Webbook
tc	753.87	K	Joback Method
tf	340.60	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.56	J/mol×K	535.50	Joback Method
cpg	325.39	J/mol×K	571.90	Joback Method

cpg	338.30	J/mol×K	608.29	Joback Method
cpg	350.35	J/mol×K	644.69	Joback Method
cpg	361.63	J/mol×K	681.08	Joback Method
cpg	372.21	J/mol×K	717.48	Joback Method
cpg	382.17	J/mol×K	753.87	Joback Method
dvisc	0.0005881	Pa×s	405.57	Joback Method
dvisc	0.0013291	Pa×s	373.08	Joback Method
dvisc	0.0035095	Pa×s	340.60	Joback Method
dvisc	0.0002937	Pa×s	438.05	Joback Method
dvisc	0.0001614	Pa×s	470.53	Joback Method
dvisc	0.0000958	Pa×s	503.02	Joback Method
dvisc	0.0000606	Pa×s	535.50	Joback Method
hvapt	62.50	kJ/mol	464.50	NIST Webbook
hvapt	56.60	kJ/mol	464.50	NIST Webbook
hvapt	54.40	kJ/mol	464.50	NIST Webbook
hvapt	49.90	kJ/mol	464.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54554e+01
Coeff. B	-4.70761e+03
Coeff. C	-8.57520e+01
Temperature range (K), min.	396.12
Temperature range (K), max.	549.83

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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=C4074435&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume